Adiabatic Vacua and Hadamard States for Scalar Quantum Fields on Curved Spacetime

arXiv:hep-th/9507097 19 Jul 1995

Dissertation
zur Erlangung des Doktorgrades
des Fachbereichs Physik
der Universität Hamburg

vorgelegt von
Wolfgang Junker
aus Weilheim/Obb.

Hamburg
1995

hep-th/9507097
DESY 95-144

Gutachter der Dissertation:	Prof. Dr. K. Fredenhagen Prof. Dr. D. Buchholz
Gutachter der Disputation:	Prof. Dr. K. Fredenhagen Prof. Dr. G. Mack
Datum der Disputation:	13. Juli 1995
Sprecher des Fachbereichs Physik und Vorsitzender des	

Promotionsausschusses: Prof. Dr. B. Kramer

Abstract

Quasifree states of a linear Klein-Gordon quantum field on globally hyperbolic spacetime manifolds are considered. Using techniques from the theory of pseudodifferential operators and wavefront sets on manifolds a criterion for a state to be an Hadamard state is developed. It is shown that ground- and KMS-states on certain static spacetimes and adiabatic vacuum states on Robertson-Walker spaces are Hadamard states. Finally, the problem of constructing Hadamard states on arbitrary curved spacetimes is solved in principle.

Zusammenfassung

Es werden quasifreie Zustände eines quantisierten linearen Klein-Gordon-Feldes auf global hyperbolischen Raumzeit-Mannigfaltigkeiten betrachtet. Unter Verwendung von Methoden aus der Theorie der Pseudodifferentialoperatoren und Wellenfrontenmengen auf Mannigfaltigkeiten wird ein Kriterium entwickelt, das es ermöglicht, die Hadamard-Eigenschaft von Zuständen nachzuweisen. Es wird gezeigt, daß Grund- und KMS-Zustände auf gewissen statischen Raumzeiten und adiabatische Vakuumzustände auf Robertson-Walker-Raumzeiten Hadamard-Zustände sind. Zu guter Letzt wird ein Konstruktionsverfahren für Hadamard-Zustände auf beliebigen gekrümmten Raumzeiten angegeben.

Contents

Chapter 1

Introduction

Hawking's remarkable discovery twenty years ago [29] that the gravitational collapse of a star to a black hole is accompanied by a thermal radiation of quantum fields at the temperature $T = 1/8\pi M$ (in natural units, M the mass of the black hole) was an essential stimulus for the investigation of quantum field theory in curved spacetime. This is a semiclassical theory in so far as the gravitational field is assumed to be given as a classical background field wherein the quantized matter fields act dynamically (for good introductions into the subject see [21, 36, 59]). The backreaction of the matter fields on the gravitational field, i.e. the spacetime metric $g_{\mu\nu}$, occurs via the semiclassical Einstein equations

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi \langle \hat{T}_{\mu\nu}(x) \rangle_\omega ,$$

where $\langle \hat{T}_{\mu\nu} \rangle_\omega$ is the expectation value of the energy-momentum tensor of the matter fields in a quantum state ω, $R_{\mu\nu}$ the Ricci tensor of $g_{\mu\nu}$ and $R = g^{\mu\nu} R_{\mu\nu}$ the Ricci scalar. As an effect of the backreaction the thermal radiation draws its energy from the gravitational field, which causes the black hole to evaporate. In a fundamental theory unifying gravity and the other forces of nature it is expected that also the metric field must be "quantized" (in some still undefined sense), nevertheless the semiclassical approximation should have validity in a large range up to the Planck scale.

One must admit that the expected effects of quantum fields in a gravitational background are very small: a black hole of ten solar masses emitts radiation at a temperature of about 10^{-8}K (which is of course concealed behind the cosmic background radiation), so only small primordial black holes or effects in the early epoch of the universe can be expected to yield observable phenomena.

On the other hand, the study of quantum field theory in curved spacetimes has already given deep insights into the interplay between quantum theory and spacetime geometry, and we think this source of physical understanding is not yet exhausted. One example is the thermodynamic behaviour of black holes which had already been noted but not understood physically before Hawking's discovery. Another is the question which rôle the global features of a spacetime play in the setting of quantum field theory. What are the local states in the absence of Poincaré symmetry? It is this question which we will mainly pursue in this work.

To this end, we consider the model of a linear scalar quantum field coupled to a gravitational background. Such a system possesses infinitely many degrees of freedom. Hence there are unitarily inequivalent representations of the canonical commutation relations and one has to pick out the physically interesting ones. For quantum fields in Minkowski space one uses the Poincaré group to specify a "vacuum state": it is the (usually unique) Poincaré-invariant state such that the translations are unitarily implementable in its GNS-Hilbertspace with a positive energy-momentum operator (spectral condition). It is the state of lowest energy, the particle states are local excitations of this vacuum state.

If we take external gravitational fields into consideration in which the quantum fields propagate one has to replace the Minkowski space by a curved spacetime manifold that does in general not possess any symmetries and we cannot expect that there exists a preferred vacuum state (this was the first time realized in [19]). The particle concept itself becomes dubious and it is probably sensible only asymptotically in regions of weak gravitational fields. In this situation the algebraic approach to quantum field theory [26, 24] is the appropriate frame to describe the physical situation. Here, one starts with a net of local algebras that contain the local observables and fields. A concrete physical realization of the system is determined by a state, i.e. a positive, linear, normalized functional on the observable algebra. It gives the expectation values of all physical quantities. Each state fixes via the GNS-construction a representation of the observable algebra on a Hilbertspace, in which it acts as a cyclic ("vacuum"-like) vector. The "folium" of a state is the set of all vector- and density matrix-states in its GNS-Hilbertspace. However, not every (mathematical) state is physically realizable. One has to select among the many unitarily inequivalent representations those which describe physically sensible situations. It was observed by Haag, Narnhofer and Stein [27, 24] that in Minkowski space all physically realizable states – when restricted to a finite, contractible spacetime region – belong to the same unique (primary) folium (namely that of the vacuum state), and they adopted this for quantum field theory on curved spacetime as a hypothesis, called the "principle of local definiteness". There is then a unique von Neumann algebra (with trivial center) which is the weak closure of all observable algebras belonging to finite, contractible regions, and the physical states are the normal states of this algebra. Two states are called locally quasiequivalent if they are normal w.r.t. this algebra, i.e. if they determine the same local folium.

Let us summarize: To make quantum field theory on curved spacetime as well defined a theory as on Minkowski space we have to specify – besides commutation relations and field equations – the folium (= quasiequivalence class) of physical states, but this folium cannot be defined as easily as in Minkowski space by appealing to the vacuum state, which does in general not exist in the presence of a gravitational field.

A second constraint on the choice of physical states is the requirement that the expectation value of the energy-momentum tensor $T_{\mu\nu}$ in a state can be regularized to become a tensorfield at a single spacetime point. This is necessary in order that the semiclassical Einstein equations make sense. In Minkowski space it is achieved by Wick ordering the fields w.r.t. the Minkowski vacuum. In curved spacetimes one has to choose the states such that certain regularization procedures can be applied.

We are concerned here with the linear Klein-Gordon quantum field on globally hyperbolic spacetimes. The corresponding algebra (with the canonical commutation relations imposed) was constructed by Dimock [13]. There are three classes of (quasifree) states on this algebra

which have been considered so far. These are
1.) the set S_1 of adiabatic vacua
2.) the set S_2 of quasifree Hadamard states
3.) the set S_3 of quasifree states possessing a scaling limit at each spacetime point that satisfies the spectral condition in the tangent space.
Let us shortly comment on their relation (the classes S_1 and S_2 will be discussed in detail in sections 3.2 and 3.4). S_3 was introduced by Haag, Narnhofer and Stein [27] (see also [17]), they show that KMS-states of this type have the correct Hawking temperature in spacetimes with horizons. Although the scaling limit assumption works even for interacting theories, the states in S_3 are in general not quasiequivalent [27], i.e. the condition is not restrictive enough. S_2 is a (proper) subset of S_3. It is known to be a local quasiequivalence class [55], but is only well defined for linear fields. It is in general very difficult, to construct states of S_2, up to now examples have only been known for spacetimes with certain symmetries. In contrast, S_1 is a large class of explicitly constructed states on cosmological spacetime models. It was shown by Lüders and Roberts [41] that S_1 forms a local folium of states. The exact relation between S_1 and S_2 has not been investigated so far. It is the aim of this work to show that in fact all adiabatic vacua are Hadamard states (i.e. $S_1 = S_2$ for linear Klein-Gordon fields on Robertson-Walker spaces) and to combine the physical ideas behind the Hadamard states and the adiabatic vacuum states to produce a construction scheme for Hadamard states on arbitrarily curved globally hyperbolic spacetimes.
We have organized this work as follows:
Chapter 2 contains a mathematical introduction into the techniques of pseudodifferential operators and wavefront sets. Since these do presently not belong to the daily applied equipment of the theoretical physicist we found it useful to give a short collection of (nearly) all mathematical material that is needed to understand our arguments in chapter 3. Most of the material is taken from [52, 31, 16], only Theorem 2.29 and Corollary 2.30 are not contained in the literature in this form. Although we tried to concentrate the facts which are spread over the literature as much as possible we did not retain from giving some of the (easier) proofs for the pedagogical benefit of the reader. Nevertheless, whoever is not interested in the mathematical side of the physical problems may skip chapter 2 altogether without hesitation and may look up a theorem or a definition when arriving at a point in chapter 3 where we refer back to it.
Chapter 3 contains the physical part of this work. In section 3.1 we present the basic setting, namely the theory of the scalar Klein-Gordon quantum field in globally hyperbolic spacetimes. In section 3.2 we review the definition of Hadamard states, its physical relevance and the new results due to Radzikowski [49] that give a local characterization of Hadamard states by the wavefront set of their two-point distributions. This is the main technical ingredient which we use in section 3.3 to prove (Theorem 3.15) that certain quasifree states of the Klein-Gordon quantum field are Hadamard states. As a first application we show that ground- and KMS-states on ultrastatic spacetimes are Hadamard states (Corollary 3.16 and Corollary 3.17). This can easily be generalized to static spacetimes possessing a timelike Killing vectorfield the norm of which is bounded from below by a positive constant. In section 3.4 we introduce – following [41] – the adiabatic vacuum states on cosmological spacetime models (Robertson-Walker spaces) and apply the techniques developed so far to prove that these all are Hadamard states

(Theorem 3.22). So the essential physical statement is (Corollary 3.23) that on these spacetimes Hadamard states and adiabatic vacua define the same local folium of states.
The problem of constructing physical states on arbitrarily curved globally hyperbolic spacetimes has found much attention in the literature, but no solution. In section 3.5 we give a counterexample to certain methods proposed in the literature by choosing a typical state from such a sample and showing (Theorem 3.25) that it does not lie in the local folium of Hadamard states. At last, in section 3.6, we solve the problem "in principle" by presenting an iteration procedure which produces an asymptotic expansion of Hadamard states in close analogy to the adiabatic vacua (Theorem 3.28).

Chapter 2

Mathematical preliminaries

2.1 Pseudodifferential operators on manifolds

Following Hörmander [31] and Taylor [52] we first introduce pseudodifferential operators on $\mathbf{R}^n$ and later, by localization, on curved manifolds. The idea is to generalize linear differential operators with variable coefficients. If $p(x,D) := \sum_{|\alpha|\leq k} a_\alpha(x) D_x^\alpha$ is a differential operator with coefficients depending on $x \in \mathbf{R}^n$, then

$$\begin{aligned} p(x,D)u(x) &= \frac{1}{(2\pi)^{n/2}} p(x,D) \int_{\mathbf{R}^n} d^n\xi \; \hat{u}(\xi) e^{ix\xi} \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} d^n\xi \; p(x,\xi)\hat{u}(\xi) e^{ix\xi}, \end{aligned} \tag{2.1}$$

with $u \in \mathcal{D}(\mathbf{R}^n)$, $\hat{u}$ its Fourier transform, $p(x,\xi) = \sum_{|\alpha|\leq k} a_\alpha(x)\xi_\alpha$ (for basic definitions and notation see the appendix).
If we replace in this expression the polynomial $p(x,\xi)$ by suitable functions $a(x,\xi)$, called *symbols*, we obtain a pseudodifferential operator. We first introduce the relevant symbol classes:

Definition 2.1 *Let X be an open subset of $\mathbf{R}^n$. Let m, ρ, δ be real numbers with $0 \leq \delta, \rho \leq 1$. Then we define the* **symbols of order** m **and type** ρ, δ *to be the set*

$$\begin{aligned} S^m_{\rho,\delta}(X \times \mathbf{R}^n) \;:=\; & \{a \in \mathcal{C}^\infty(X \times \mathbf{R}^n);\ \textit{for every compact } K \subset X \textit{ and for all multiindices } \alpha, \beta \\ & \exists C_{\alpha,\beta,K} \in \mathbf{R} : \left| D_x^\beta D_\xi^\alpha a(x,\xi) \right| \leq C_{\alpha,\beta,K}(1+|\xi|)^{m-\rho|\alpha|+\delta|\beta|} \\ & \textit{for } x \in K,\ \xi \in \mathbf{R}^n\}. \end{aligned} \tag{2.2}$$

(We also simply write $S^m_{\rho,\delta}$ if no confusion is possible).
$S^{-\infty} := \bigcap_m S^m_{\rho,\delta} = \bigcap_m S^m_{1,0}$.

In the physical applications in the next chapter we only have to deal with symbols (and pseudodifferential operators) of type 1,0. Nevertheless, we keep the discussion in this mathematical introduction more general because it costs no more effort and makes the comparison with the mathematical literature easier.

Lemma 2.2 *Let* $a \in S^m_{\rho,\delta}(X \times \mathbf{R}^n), b \in S^{m'}_{\rho',\delta'}(X \times \mathbf{R}^n)$. *Then*
a) $ab \in S^{m+m'}_{\rho'',\delta''}$, *where* $\rho'' := \min(\rho, \rho'), \delta'' := \max(\delta, \delta')$,
b) $D^\beta_x D^\alpha_\xi a \in S^{m-\rho|\alpha|+\delta|\beta|}_{\rho,\delta}$,
c) If $|a(x,\xi)| \leq C(1+|\xi|)^{-m}$, *then* $a(x,\xi)^{-1} \in S^{-m}_{\rho,\delta}$.
d) $\chi \in \mathcal{C}^\infty_o(\mathbf{R}^n) \Rightarrow \chi a \in S^{-\infty}$. *This implies that a symbol changes only by a term in* $S^{-\infty}$ *if we modify it in a compact domain in* ξ.

The proof follows easily from the chain rule.
Before introducing pseudodifferential operators we give the notion of the **asymptotic expansion** of a symbol. It is an important tool for the construction of certain pseudodifferential operators (as used e.g. in Theorem 2.16) and will have an essential application in section 3.6:

Lemma 2.3 *Suppose* $a_j \in S^{m_j}_{\rho,\delta}(X \times \mathbf{R}^n), m_j \downarrow -\infty$ $(j = 0, 1, 2, \ldots)$.
Then there exists $a \in S^{m_o}_{\rho,\delta}(X \times \mathbf{R}^n)$ *such that for all* $N > 0$:

$$a - \sum_{j=0}^{N-1} a_j \in S^{m_N}_{\rho,\delta}(X \times \mathbf{R}^n). \tag{2.3}$$

The function a *is uniquely determined modulo* $S^{-\infty}(X \times \mathbf{R}^n)$.
If (2.3) holds we write $a \sim \sum_{j\geq 0} a_j$.

PROOF:
i) Pick compact sets K_i with $K_1 \subset K_2 \subset \ldots \to X$.
Take $\psi \in \mathcal{C}^\infty(\mathbf{R}^n)$ with $\psi(\xi) = \begin{cases} 0, & |\xi| \leq 1 \\ 1, & |\xi| \geq 2 \end{cases}$, $0 \leq \psi(\xi) \leq 1$.
Choose $\epsilon_j, j = 0, 1, 2, \ldots$, such that $1 \geq \epsilon_o > \epsilon_1 \ldots > \epsilon_j \to 0$ $(j \to \infty)$ and set

$$a(x,\xi) := \sum_{j=0}^{\infty} \psi(\epsilon_j \xi) a_j(x,\xi). \tag{2.4}$$

Note that

$$\psi(\epsilon\xi) = \begin{cases} 0, & |\xi| \leq 1/\epsilon \\ 1, & |\xi| \geq 2/\epsilon \end{cases}, \tag{2.5}$$

hence, for $|\xi| \leq 1/\epsilon$ or $|\xi| \geq 2/\epsilon$, $D^\alpha_\xi \psi(\epsilon\xi) = 0$ $(\alpha \neq 0)$, whereas, if $1/\epsilon < |\xi| < 2/\epsilon$ for $0 < \epsilon \leq 1$, then $\epsilon \leq 2/|\xi| \leq 4(1+|\xi|)^{-1}$ and, since ψ varies only over a compact interval,

$$|D^\alpha_\xi \psi(\epsilon\xi)| \leq C_\alpha \epsilon^{|\alpha|} \leq C'_\alpha (1+|\xi|)^{-|\alpha|}$$

for $\alpha \neq 0$ (C_α independent of ϵ).
Thus, $\psi(\epsilon\xi) \in S^0_{1,0} \subset S^0_{\rho,\delta}$ for $0 < \epsilon \leq 1$.
So, by Lemma 2.2, for any i, j and any $0 < \epsilon \leq 1$ we have for all $x \in K_i$:

$$\begin{aligned} |D^\alpha_\xi D^\beta_x \psi(\epsilon\xi) a_j(x,\xi)| &\leq C_{i,j,\alpha,\beta}(1+|\xi|)^{m_j-\rho|\alpha|+\delta|\beta|} \\ &\leq \left[C_{i,j,\alpha,\beta}(1+|\xi|)^{-1}\right](1+|\xi|)^{m_j+1-\rho|\alpha|+\delta|\beta|}. \end{aligned} \tag{2.6}$$

Now determine $\epsilon_j > 0$ such that $C_{i,j,\alpha,\beta}\epsilon_j \leq 2^{-j}$ for $|\alpha| + |\beta| + i \leq j$.
If $(1+|\xi|)^{-1} \geq \epsilon_j$, then $|\xi| \leq 1 + |\xi| \leq 1/\epsilon_j$ and, by (2.5), $\psi(\epsilon_j\xi) = 0$.
On the other hand, if $(1+|\xi|)^{-1} \leq \epsilon_j$, we have from (2.6)

$$|D_\xi^\alpha D_x^\beta(\psi(\epsilon_j\xi)a_j(x,\xi))| \leq 2^{-j}(1+|\xi|)^{m_j+1-\rho|\alpha|+\delta|\beta|} \tag{2.7}$$

for $x \in K_i$ and $|\alpha| + |\beta| + i \leq j$. The sum in (2.4) is finite for any (x,ξ), and since $\sum_{j=0}^\infty |D_\xi^\alpha D_x^\beta(\psi(\epsilon_j\xi)a_j(x,\xi))| < \infty$ by (2.7), we have $a(x,\xi) \in \mathcal{C}^\infty(X \times \mathbf{R}^n)$.
ii) Given α, β and $x \in K_i$ we choose k so large that $|\alpha| + |\beta| + i \leq k$ and $m_k + 1 \leq m_o$ and write

$$\begin{aligned}
|D_\xi^\alpha D_x^\beta a(x,\xi)| &\leq \left|D_\xi^\alpha D_x^\beta \sum_{j=0}^{k-1} \psi(\epsilon_j\xi)a_j(x,\xi)\right| + \left|D_\xi^\alpha D_x^\beta \sum_{j=k}^{\infty} \psi(\epsilon_j\xi)a_j(x,\xi)\right| \\
&\overset{(2.6)(2.7)}{\leq} C_{\alpha,\beta,i}(1+|\xi|)^{m_o-\rho|\alpha|+\delta|\beta|} + \underbrace{\left(\sum_{j=k}^{\infty} 2^{-j}\right)}_{\leq 1}(1+|\xi|)^{m_o-\rho|\alpha|+\delta|\beta|} \\
&\leq C'_{\alpha,\beta,i}(1+|\xi|)^{m_o-\rho|\alpha|+\delta|\beta|}.
\end{aligned}$$

Since this holds for any α, β, we have $a(x,\xi) \in S_{\rho,\delta}^{m_o}$.
iii) Similarly, for any $N \in \mathbf{N}$ we obtain $\sum_{j=N}^\infty \psi(\epsilon_j\xi)a_j \in S_{\rho,\delta}^{m_N}$ and $\sum_{j=0}^{N-1}(\psi(\epsilon_j\xi)-1)a_j \in S^{-\infty}$, since $\psi(\epsilon_j\xi) - 1 = 0$ for $j \leq N-1$ and $|\xi| \geq 2/\epsilon_{N-1}$ (equ. (2.5)), and hence

$$\begin{aligned}
a - \sum_{j=0}^{N-1} a_j &= \sum_{j=0}^{N-1}(\psi(\epsilon_j\xi)-1)a_j + \sum_{j=N}^{\infty}\psi(\epsilon_j\xi)a_j \\
&\in S_{\rho,\delta}^{m_N} \quad \text{for any } N,
\end{aligned}$$

which proves (2.3).
iv) Let $b \in S_{\rho,\delta}^{m_o}(X \times \mathbf{R}^n)$ be another symbol with property (2.3), then

$$a - b = \left(a - \sum_{j=0}^{N-1} a_j\right) - \left(b - \sum_{j=0}^{N-1} a_j\right) \in S_{\rho,\delta}^{m_N},$$

for all $N > 0$, hence $a = b\,(mod\ S^{-\infty})$. □

Definition 2.4 *If $a(x,\xi) \in S_{\rho,\delta}^m(X \times \mathbf{R}^n)$ the operator*

$$Au(x) := \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} e^{ix\eta}a(x,\eta)\hat{u}(\eta)\, d^n\eta, \tag{2.8}$$

$u \in \mathcal{S}(\mathbf{R}^n), x \in X$, is said to belong to $L_{\rho,\delta}^m(X)$, the **pseudodifferential operators** *of type ρ, δ (we drop the X and write $L_{\rho,\delta}^m$ when the context is clear).*

Examples:

1. Let $A := \sum_{|\alpha|\leq m} a_\alpha(x)D_x^\alpha, a_\alpha \in \mathcal{C}^\infty(X)$, be a linear partial differential operator of order m on $X \subset \mathbf{R}^n$. Then $A \in L_{1,0}^m(X)$.

2. Let $(Au)(x) := \int_{\mathbf{R}^n} K(x,y)u(y)\, d^n y$ with $K \in \mathcal{C}^\infty(X \times X)$ such that $supp K(x,\cdot)$ is compact for each $x \in X$.
   Then $A \in L^{-\infty}(X)$. [The symbol is $a(x,\xi) = \int_{\mathbf{R}^n} K(x,y)e^{i(y-x)\xi}\, d^n y$, i.e. the Fourier transform of a function with compact support and hence rapidly decreasing in ξ.]
   In particular the convolution $u \mapsto u * \varphi := \int_{\mathbf{R}^n} \varphi(x-y)u(y)\, d^n y$ with $\varphi \in \mathcal{C}_o^\infty(X)$ is such a pseudodifferential operator. We remark that in this case $supp\, Au = supp\, u + supp\, \varphi$.

3. Let A denote the multiplication with $\chi \in \mathcal{C}_o^\infty(X): \quad (Au)(x) := \chi(x)u(x)$.
   Then $A \in L^0_{1,0}(X)$.

The properties of A as an operator are given in the following theorem.

Theorem 2.5 *a) $A \in L^m_{\rho,\delta}(X)$ is a continuous operator $A : \mathcal{D}(X) \to \mathcal{C}^\infty(X)$.*
b) If $\delta < 1$, then the map can be extended to a continuous map $A : \mathcal{E}'(X) \to \mathcal{D}'(X)$.

PROOF:
a) Let $a \in S^m_{\rho,\delta}(X \times \mathbf{R}^n), u \in \mathcal{D}(X)$. Since $\hat{u} \in \mathcal{S}(X)$ the integral
$Au(x) = (1/2\pi)^{n/2} \int a(x,\xi)\hat{u}(\xi)e^{ix\xi}\, d^n\xi$ is absolutely convergent, and one can differentiate under the integral sign, obtaining always absolutely convergent integrals because of (2.2).
b) We show that the functional $v \mapsto \langle Au, v\rangle,\ v \in \mathcal{D}(X)$, is well defined for $u \in \mathcal{E}'(X)$: Formally

$$\begin{aligned} \langle Au, v\rangle &= \frac{1}{(2\pi)^{n/2}} \iint v(x)a(x,\xi)\hat{u}(\xi)e^{ix\xi}\, d^n\xi\, d^n x \\ &= \frac{1}{(2\pi)^{n/2}} \int a_v(\xi)\hat{u}(\xi)\, d^n\xi \qquad (2.9) \\ \text{with} \quad a_v(\xi) &:= \int v(x)a(x,\xi)e^{ix\xi}\, d^n x. \end{aligned}$$

Since the Fourier transform $\hat{u}$ of a distribution u with compact support can at most grow polynomially (2.9) is well defined for any $u \in \mathcal{E}'(X)$ if $a_v(\xi)$ is rapidly decreasing:
Integration by parts yields for $\eta, \xi \in \mathbf{R}^n$:

$$\begin{aligned} \left|\eta^\alpha \int v(x)a(x,\xi)e^{ix\eta}\, d^n x\right| &= \left|\int D_x^\alpha(v(x)a(x,\xi))e^{ix\eta}\, d^n x\right| \\ &\leq \int |D_x^\alpha(v(x)a(x,\xi))|\, d^n x \\ &\leq C_\alpha(1+|\xi|)^{m+\delta|\alpha|} \quad \text{by (2.2)} \\ \Rightarrow \left|\int v(x)a(x,\xi)e^{ix\eta}\, d^n x\right| &\leq C_N(1+|\xi|)^{m+\delta N}(1+|\eta|)^{-N}, \\ \text{hence, for } \xi = \eta\text{:} \quad |a_v(\xi)| &\leq C_N(1+|\xi|)^{m+(\delta-1)N}. \end{aligned}$$

If $\delta < 1$, this implies the rapid decrease of $a_v(\xi)$. □

Since A is continuous it is given by a distribution kernel $K_A \in \mathcal{D}'(X \times X)$ via $\langle Au, v\rangle = \langle K_A, u \otimes v\rangle$ for $u, v \in \mathcal{D}(X)$ (Schwartz' kernel theorem).

Lemma 2.6 *a) If $A \in L^m_{\rho,\delta}(X)$ for $\rho > 0$, then K_A is $\mathcal{C}^\infty$ off the diagonal in $X \times X$.*
b) If $A \in L^{-\infty}(X)$, then K_A is smooth everywhere in $X \times X$ (which is the converse of Example 2) above).

PROOF:
Let $u, v \in \mathcal{D}(X)$. We have

$$\begin{aligned}\langle K_A, u \otimes v\rangle &= \langle Au, v\rangle = \int v(x) Au(x)\, d^n x = \\ &= \frac{1}{(2\pi)^{n/2}} \iint a(x,\xi) e^{ix\xi} v(x) \hat{u}(\xi)\, d^n\xi\, d^n x = \\ &= \frac{1}{(2\pi)^n} \iiint a(x,\xi) e^{i(x-y)\xi} v(x) u(y)\, d^n y\, d^n\xi\, d^n x.\end{aligned}$$

Thus

$$K_A(x,y) = \frac{1}{(2\pi)^n} \int a(x,\xi) e^{i(x-y)\xi}\, d^n\xi$$

as a distribution integral. In this sense it follows after partial integration

$$|(x-y)^\alpha K_A(x,y)| = \left| \frac{1}{(2\pi)^n} \int e^{i(x-y)\xi} D_\xi^\alpha a(x,\xi)\, d^n\xi \right|,$$

which converges absolutely by (2.2) if $m - \rho|\alpha| < -n$. Furthermore,

$$\left| D_x^\beta D_y^\gamma (x-y)^\alpha K_A(x,y) \right| = \left| \frac{1}{(2\pi)^n} \int D_x^\beta D_y^\gamma e^{i(x-y)\xi} D_\xi^\alpha a(x,\xi)\, d^n\xi \right|$$

converges absolutely if $m - \rho|\alpha| + \delta|\beta| < -n - |\beta| - |\gamma|$. Since $|\alpha|$ can be made arbitrarily large this shows that $K_A(x,y)$ is smooth for $x \neq y$. If m can be chosen arbitrarily negative, absolute convergence holds even for $|\alpha| = 0$, i.e. K_A is smooth everywhere. □

Definition 2.7 *A distribution $u \in \mathcal{D}'(X \times X)$ is called* **properly supported** *if $\{(x,y) \in$ supp $u;\ x \in K$ or $y \in K\}$ is compact for every compact set $K \subset X$, i.e. supp u has compact intersection with $K \times X$ and $X \times K$. Equivalently, u is properly supported if for each compact $K \subset X$ there exists a compact $K' \subset X$ such that*

$$\begin{aligned} \text{supp}\, f \subset K \quad &\Rightarrow \quad \text{supp}\, uf \subset K' \\ \text{and } f = 0 \text{ on } K' \quad &\Rightarrow \quad uf = 0 \text{ on } K. \end{aligned} \tag{2.10}$$

A pseudodifferential operator A is called properly supported if its distribution kernel K_A is properly supported.

From Theorem 2.5 it follows that, if A is properly supported, then $A : \mathcal{C}^\infty(X) \to \mathcal{C}^\infty(X)$ and $A : \mathcal{D}'(X) \to \mathcal{D}'(X)$ (for $\delta < 1$).
Every pseudodifferential operator A can be written as the sum of one with a $\mathcal{C}^\infty$-kernel and one which is properly supported. To this end, we choose a $\chi \in \mathcal{C}^\infty(X \times X)$ such that $\chi = 1$ in a neighborhood of the diagonal and χ is properly supported. By writing $K_A = (1-\chi)K_A + \chi K_A$ we obtain the desired splitting: $(1-\chi)K_A$ is smooth because of Lemma 2.6a) and χK_A is properly supported since χ is so.
Thus, in the following, we can always assume that pseudodifferential operators are properly supported. This has the advantage that for these there exists a simple calculus:

Two pseudodifferential operators $A \in L^m_{\rho,\delta}$ and $B \in L^{m'}_{\rho,\delta}$ (with symbols $a(x,\xi)$ resp. $b(x,\xi)$, say) can be composed yielding again a pseudodifferential operator (in $L^{m+m'}_{\rho,\delta}$) with symbol

$$\sigma_{AB}(x,\xi) \sim \sum_{\alpha\geq 0} \frac{i^{|\alpha|}}{\alpha!}(D^\alpha_\xi a(x,\xi))(D^\alpha_x b(x,\xi)), \tag{2.11}$$

and there exists the adjoint A^t resp. $A^* \in L^m_{\rho,\delta}$ of a pseudodifferential operator $A \in L^m_{\rho,\delta}$ (defined by $(Au,v) = (u, A^t v)$ resp. $(Au,v) = (u, A^* v)$ for the scalar product in $L^2_{\mathbf{R}}(\mathbf{R}^n, \sqrt{h} d^n x)$ resp. $L^2_{\mathbf{C}}(\mathbf{R}^n, \sqrt{h} d^n x)$, $h \in \mathcal{C}^\infty(\mathbf{R}^n)$) with symbol

$$\begin{aligned} \sigma_{A^t}(x,\xi) &\sim \sum_{\alpha\geq 0} \frac{i^{|\alpha|}}{\alpha! h(x)^{1/2}} D^\alpha_\xi D^\alpha_x \left[h(x)^{1/2} a(x,-\xi)\right] \\ \sigma_{A^*}(x,\xi) &\sim \sum_{\alpha\geq 0} \frac{i^{|\alpha|}}{\alpha! h(x)^{1/2}} D^\alpha_\xi D^\alpha_x \left[h(x)^{1/2}\overline{a(x,\xi)}\right]. \end{aligned} \tag{2.12}$$

Note in particular that

$$\begin{aligned} \sigma_{AB}(x,\xi) - a(x,\xi)b(x,\xi) &\in S^{m+m'-(\rho-\delta)}_{\rho,\delta} \\ \sigma_{A^t}(x,\xi) - a(x,-\xi) &\in S^{m-(\rho-\delta)}_{\rho,\delta} \\ \sigma_{A^*}(x,\xi) - \overline{a(x,\xi)} &\in S^{m-(\rho-\delta)}_{\rho,\delta}. \end{aligned} \tag{2.13}$$

For details see [52, section II§4] or [31, section 2.1].
For us, the most important aspect is the effect of a change of variables on a properly supported pseudodifferential operator. It will allow to give these operators a well defined meaning on a curved manifold.
Let X and Y be open regions in $\mathbf{R}^n$ and $\kappa : X \to Y$ a diffeomorphism. Let $A \in L^m_{\rho,\delta}(X)$ with symbol $a(x,\xi)$ and set

$$\tilde{A}u := (A(u\circ\kappa))\circ\kappa^{-1}, \quad u \in \mathcal{C}^\infty_o(Y),$$

so $\tilde{A} : \mathcal{C}^\infty_o(Y) \to \mathcal{C}^\infty(Y)$.
The following main theorem shows that $\tilde{A}$ is also a pseudodifferential operator and gives the transformation law for the symbol:

Theorem 2.8 *If $A \in L^m_{\rho,\delta}(X)$ is properly supported and if $\rho > 1/2$ and $\rho+\delta \geq 1$, then $\tilde{A} \in L^m_{\rho,\delta}(Y)$ with symbol*

$$\tilde{a}(\kappa(x),\xi) \sim \sum_{\alpha\geq 0} \frac{1}{\alpha!}\varphi_\alpha(x,\xi) D^\alpha_\xi a(x, {}^t\kappa'(x)\xi), \tag{2.14}$$

where $\varphi_\alpha(x,\xi) := D^\alpha_y \exp i\langle(\kappa(y)-\kappa(x)-\kappa'(x)(y-x)),\xi\rangle|_{x=y}$ is a polynomial in ξ of degree $\leq |\alpha|/2$, in particular

$$\begin{aligned} \varphi_o(x,\xi) &= 1, \quad \varphi_\alpha(x,\xi) = 0 \quad \textit{for } |\alpha| = 1, \\ \varphi_\alpha(x,\xi) &= iD^\alpha_x\langle\kappa(x),\xi\rangle \quad \textit{for } |\alpha| = 2. \end{aligned}$$

Here κ' denotes the Jacobian $\frac{D\kappa(x)}{Dx}$ of κ and ${}^t\kappa'$ its transpose.

The proof uses as a main technical tool a new integral representation for pseudodifferential operators, which we do not want to introduce here. Therefore we refer the interested reader to [52, II§5].
Up to now we have considered pseudodifferential operators on $\mathbf{R}^n$ as determined modulo operators in $L^{-\infty}$ and symbols in $S^{-\infty}$. Formula (2.14) however suggests a different point of view if we are on a manifold: The terms of index $\alpha \neq 0$ in the sum of equ. (2.14) are of order $\leq m - \rho|\alpha| + |\alpha|/2 = m - |\alpha|(\rho - \frac{1}{2}) \leq m - (2\rho - 1) < m$ for $\rho > 1/2$ and $\rho + \delta \geq 1$. We can define equivalence classes $L^m_{\rho,\delta}(X)/L^{m-(2\rho-1)}_{\rho,\delta}(X)$ of pseudodifferential operators, i.e. we consider two operators as equivalent if they differ by an operator of order $\leq m - (2\rho - 1)$.

Definition 2.9 *If $A \in L^m_{\rho,\delta}(X)$ we define the* **principal symbol** *of A to be a member in the corresponding equivalence class $S^m_{\rho,\delta}(X \times \mathbf{R}^n)/S^{m-(2\rho-1)}_{\rho,\delta}(X \times \mathbf{R}^n)$.*

The decisive point now is the following: From equ. (2.14) we observe that if $\tilde{A}$ is obtained from A (having symbol $a(x,\xi)$) by a change κ of coordinates as discussed above, then a principal symbol of $\tilde{A}$ is given by

$$a(\kappa^{-1}(x), {}^t\kappa'(x)\xi), \tag{2.15}$$

i.e. the principal symbol is a well defined function on the cotangent bundle $T^*\mathcal{M}$ of a manifold $\mathcal{M}$.
In a similar way we obtain from (2.13) the principal symbol of the adjoint A^t resp. A^* as $a(x,-\xi)$ resp. $\overline{a(x,\xi)}$ and if $b(x,\xi)$ is a principal symbol of B then $a(x,\xi)b(x,\xi)$ is a principal symbol of AB. (This, by the way, means that pseudodifferential operators commute in highest order.)
The fact that the principal symbols form a well defined $*$-algebra of functions on the cotangent bundle $T^*\mathcal{M}$ makes pseudodifferential operators such a useful tool for analysis on curved manifolds. We are now naturally led to define:

Definition 2.10 *Let $\mathcal{M}$ be a $\mathcal{C}^\infty$ paracompact manifold of dimension n.
For $\rho > 1/2$ and $\rho + \delta \geq 1$ we define $L^m_{\rho,\delta}(\mathcal{M})$ to be the space of continuous linear operators $A : \mathcal{C}^\infty_o(\mathcal{M}) \to \mathcal{C}^\infty(\mathcal{M})$ with the property that for each diffeomorphism κ of a coordinate patch $X_\kappa \subset \mathcal{M}$ to an open set $\kappa X_\kappa \subset \mathbf{R}^n$ we have $A_\kappa \in L^m_{\rho,\delta}(\kappa X_\kappa)$, where $A_\kappa u := (A(u \circ \kappa)) \circ \kappa^{-1}$ for $u \in \mathcal{C}^\infty_o(\kappa X_\kappa)$.*

It is sufficient to require that this condition is verified for a covering of $\mathcal{M}$ by coordinate patches if in addition we require that K_A is smooth off the diagonal in $\mathcal{M} \times \mathcal{M}$. It is also equivalent to the following condition: if $x^1, \ldots, x^n$ are local coordinates in an open coordinate patch $X \subset \mathcal{M}$ and if $v \in \mathcal{C}^\infty_o(X)$, then

$$e^{-ix\xi} A\left(ve^{ix\xi}\right) \in S^m_{\rho,\delta}(X \times \mathbf{R}^n), \tag{2.16}$$

where $\xi \in \mathbf{R}^n,\ x\xi := x^1\xi_1 + \ldots + x^n\xi_n$.
Of course, the theorems and lemmata proven above remain valid locally on a manifold.

2.2 Wavefront sets of distributions

The notion of the wavefront set of a distribution has been introduced by Hörmander [31]. It will be the main tool to characterize two-point functions of quasifree states of a quantum field, as will be explained in the next chapter. Therefore we have to introduce this concept, its connection with pseudodifferential operators and the calculus related to it.

Definition 2.11 *Let $X \subset \mathcal{M}$ be a coordinate patch with coordinates (x, ξ) of $T^*\mathcal{M}$. If $u \in \mathcal{D}'(X)$ the* **wavefront set** *$WF(u)$ is the set*

$$WF(u) := \bigcap_{\substack{A \in L^0_{1,0} \\ Au \in \mathcal{C}^\infty}} char\ A \tag{2.17}$$

where

$$char\ A := \{(x, \xi) \in T^*X \setminus \{0\}; \liminf_{t \to \infty} |a(x, t\xi)| = 0\} \tag{2.18}$$

is the **characteristic set** *of a properly supported pseudodifferential operator A with principal symbol $a(x, \xi)$ (the choice of principal symbol is irrelevant in the definition).*

The most important properties of wavefront sets are the following:
1) Let $u \in \mathcal{D}'(X)$. $\forall \varphi \in \mathcal{C}^\infty_o(X)$: $WF(\varphi u) \subset WF(u)$, and $(x_o, \xi_o) \in WF(u) \Leftrightarrow (x_o, \xi_o) \in WF(\varphi u)$ when $\varphi(x_o) \neq 0$.
This shows that the wavefront set is a local object depending only on arbitrarily small neighborhoods of points $x_o \in X$.
2) We observed in the last section that a principal symbol of a pseudodifferential operator transforms covariantly under diffeomorphisms. Therefore by the Definition (2.17) $WF(u)$ is a well defined subset of the cotangential bundle $T^*\mathcal{M}$ of a manifold $\mathcal{M}$, i.e. if $\kappa : X \to Y$ is a diffeomorphism between open coordinate patches $X, Y \subset \mathbf{R}^n$ of a manifold $\mathcal{M}$, $u \in \mathcal{D}'(Y)$ and $\tilde{u} \in \mathcal{D}'(X)$ the distribution with $\tilde{u}(f) := u(f \circ \kappa^{-1})$ for $f \in \mathcal{D}(X)$ then

$$WF(\tilde{u}) = \kappa_* WF(u) := \{(\kappa^{-1}(x), {}^t\kappa'(x)\xi);\ (x, \xi) \in WF(u)\}.$$

Because of property 1) we can define the wavefront set of a distribution on a manifold just by localization on coordinate patches.
3) $WF(u)$ is a closed cone in $T^*\mathcal{M} \setminus \{0\}$, i.e. $(x, \xi) \in WF(u)$ implies $(x, t\xi) \in WF(u)$ for all $t > 0$.
4) The wavefront set is a refinement of the notion of singular support of a distribution in the following sense:

Theorem 2.12 *Let $\pi : T^*\mathcal{M} \to \mathcal{M}$ denote the projection of $T^*\mathcal{M}$ onto its base space. Then*

$$\pi(WF(u)) = singsupp\, u. \tag{2.19}$$

In particular, the wavefront set is empty if u is smooth.

PROOF:
i) $x_o \notin singsupp\, u \Rightarrow \exists \varphi \in \mathcal{C}_o^\infty(X),\ \varphi = 1$ near x_o such that $\varphi u \in \mathcal{C}_o^\infty(X)$.
Clearly $(x_o, \xi) \notin char\, \varphi \supset WF(u)$ for any $\xi \neq 0$, hence $\pi(WF(u)) \subset singsupp\, u$.
ii) $x_o \notin \pi(WF(u)) \Rightarrow \forall \xi \neq 0\ \exists A \in L^0_{1,0}$ such that $(x_o, \xi) \notin char\, A$ and $Au \in \mathcal{C}^\infty$.
Thus there exist finitely many $A_j \in L^0_{1,0}$ such that $A_j u \in \mathcal{C}^\infty$ and each (x_o, ξ), $|\xi| = 1$, is noncharacteristic for some A_j.
Let $B := \sum_j A_j^* A_j \in L^0_{1,0}$. Then B is elliptic near x_o and $Bu \in \mathcal{C}^\infty$, so – by the following Theorem 2.16 – u is $\mathcal{C}^\infty$ near x_o, which shows that $singsupp\, u \subset \pi(WF(u))$. □
5)

$$WF(u_1 + u_2) \subset WF(u_1) \cup WF(u_2) \tag{2.20}$$

6) Differential operators P are in an essential way characterized by their locality property, namely that always $supp\,(Pu) \subset supp\, u$. For pseudodifferential operators this is in general no longer true (see Example 2) in the previous section), but there is a remnant of it, the so-called **pseudolocal property**:

Theorem 2.13 (Theorem 1.6 of [52]) *Let $A \in L^m_{\rho,\delta}(\mathcal{M})$ for $\rho > 0$ and $u \in \mathcal{D}'(\mathcal{M})$. Then*

$$WF(Au) \subset WF(u). \tag{2.21}$$

An important application of pseudodifferential operators is the treatment of elliptic (differential) equations. One result in this direction which we need later on is easy to state and very instructive to prove:

Definition 2.14 *An operator $A \in L^m_{\rho,\delta}(X)$ is* **elliptic of order** *m if on each compact $K \subset X$ there are constants C_K and R such that for its symbol*

$$|a(x,\xi)| \geq C_K |\xi|^m \quad \text{for } x \in K,\ |\xi| > R. \tag{2.22}$$

Because of the transformation law (2.15) of the principal symbol of A under diffeomorphisms the property of ellipticity is invariant under diffeomorphisms, and we define a pseudodifferential operator on a manifold $\mathcal{M}$ to be elliptic if it is so in any local chart.

Example:
The Laplace-Beltrami operator on a Riemannian manifold is an elliptic (pseudo-)differential operator of order 2.
The next theorem states that such operators can be inverted "up to $L^{-\infty}$". This is done by the construction of so-called parametrices.

Definition 2.15 *Let A be a properly supported pseudodifferential operator on a manifold $\mathcal{M}$. If Q is a continuous mapping $\mathcal{C}_o^\infty(\mathcal{M}) \to \mathcal{C}^\infty(\mathcal{M})$ such that i) $QA = I + R_1$, ii) $AQ = I + R_2$ or iii) $QA = AQ = I + R_3$, where R_i have smooth kernels and I is the identity operator, then we call Q a i)* **left**, *ii)* **right** *or iii)* **two-sided parametrix** *of A. (For a two-sided parametrix we often simply say "parametrix".)*

Theorem 2.16 *If $A \in L^m_{\rho,\delta}(X)$, $\rho > \delta$, is a properly supported elliptic pseudodifferential operator of order m, then there is a properly supported parametrix $Q \in L^{-m}_{\rho,\delta}(X)$ which is elliptic of order $-m$. It follows that*

$$WF(u) = WF(Au) \quad \textit{for}\, u \in \mathcal{D}'(X). \tag{2.23}$$

PROOF:
If Q has the desired properties we have

$$u = (I - QA)u + QAu = Ru + QAu,$$

where R has smooth kernel, and, using Theorem 2.13,

$$WF(u) \subset WF(QAu) \subset WF(Au) \subset WF(u),$$

from which (2.23) follows.
Therefore it remains to construct Q which we do by successive approximations. If $a(x,\xi)$ is the symbol of A we set

$$q_o(x,\xi) := \chi(x,\xi)a(x,\xi)^{-1}$$

where $\chi = 0$ in a neighborhood of the zeros of a and χ is identically 1 for large ξ (there, a cannot have zeros because of condition (2.22)). Hence, because of Lemma 2.2c)

$$q_o \in S^{-m}_{\rho,\delta}(X \times \mathbf{R}^n).$$

Let $Q_o \in L^{-m}_{\rho,\delta}(X)$ with symbol q_o, then Q_oA has symbol $\chi(x,\xi) + r(x,\xi)$ with $r(x,\xi) \in S^{-(\rho-\delta)}_{\rho,\delta}(X \times \mathbf{R}^n)$, and since $\chi - 1 \in S^{-\infty}$ we have

$$Q_oA = I + R, \quad R \in L^{-(\rho-\delta)}_{\rho,\delta}(X).$$

Now we define $E \in L^0_{\rho,\delta}(X)$ to have the asymptotic expansion

$$E \sim I - R + R^2 - R^3 + \dots$$

(in the sense of Lemma 2.3), then

$$(EQ_o)A = I + K_1, \quad K_1 \in L^{-\infty}.$$

Consequently, $Q := EQ_o \in L^{-m}_{\rho,\delta}$ is a left parametrix of A.
Similarly we can construct a right parametrix $\tilde{Q}$ of A, namely, with

$$AQ_o = I + \tilde{R}, \quad \tilde{R} \in L^{-(\rho-\delta)}_{\rho,\delta},$$

take

$$\tilde{E} \sim I - \tilde{R} + \tilde{R}^2 - \tilde{R}^3 + \dots,$$

hence

$$A(Q_0\tilde{E}) = I + K_2, \quad K_2 \in L^{-\infty},$$

and let $\tilde{Q} := Q_o \tilde{E} \in L^{-m}_{\rho,\delta}(X)$.
Therefore we have

$$\begin{aligned} QA\tilde{Q} &= (I+K_1)\tilde{Q} = \tilde{Q} + K_1\tilde{Q} \quad \text{and} \\ QA\tilde{Q} &= Q(I+K_2) = Q + QK_2, \quad \text{hence} \\ Q - \tilde{Q} &= K_1\tilde{Q} - QK_2 \in L^{-\infty}(X), \end{aligned}$$

i.e. $Q = \tilde{Q} \; mod \, L^{-\infty}(X)$ is a two-sided parametrix.
If q is a principal symbol of Q, then $QA = \chi$ is a principal symbol of QA. Since $a \in S^m_{\rho,\delta}$ we have for $x \in K \subset X$ and large ξ

$$|q(x,\xi)| = |\chi(x,\xi)a(x,\xi)^{-1}| \geq C_K(1+|\xi|)^{-m},$$

i.e. Q is elliptic of order $-m$. □

(2.23) is a special property of elliptic operators. For hyperbolic operators (e.g. the Klein-Gordon operator, which plays a prominent rôle in this work) the behaviour of wavefront sets is more complicated. It is determined by the following important theorem on the **propagation of singularities** which we will repeatedly apply in connection with the Klein-Gordon operator.

Theorem 2.17 (Theorem 6.1.1. of [16]) *Let $A \in L^m_{1,0}(\mathcal{M})$ be a properly supported pseudo-differential operator with real principal symbol a which is homogeneous of degree m.*
If $u \in \mathcal{D}'(\mathcal{M})$ and $Au = f$ it follows that

$$WF(u) \setminus WF(f) \subset a^{-1}(0) \setminus \{0\} \tag{2.24}$$

and $WF(u) \setminus WF(f)$ is invariant under the Hamiltonian vector field H_a given by

$$H_a := \sum_{i=1}^{n} \left[\frac{\partial a(x,\xi)}{\partial x^i} \frac{\partial}{\partial \xi_i} - \frac{\partial a(x,\xi)}{\partial \xi_i} \frac{\partial}{\partial x^i} \right] \tag{2.25}$$

in local coordinates.

Remarks:
This theorem contains as special cases two properties which we have already learnt of:

1. If $a^{-1}(0) \setminus \{0\} = \emptyset$, i.e. A is elliptic, then $WF(u) \subset WF(Au) \subset WF(u)$ by (2.24) and (2.21), which was the result of Theorem 2.16.

2. If Au is a smooth function, i.e. $WF(Au) = \emptyset$, then by (2.24) $WF(u) \subset a^{-1}(0) \setminus \{0\}$, which is already contained in the Definition (2.17) of the wavefront set. In this definition one can replace $A \in L^0_{1,0}$ by $A \in L^q_{1,0}$ for any $q \in \mathbf{R}$, because for a pseudodifferential operator $A \in L^0_{1,0}$ and an elliptic one $B \in L^q_{1,0}$, $char\,(BA) = char\,(A)$ and $Au \in \mathcal{C}^\infty \Leftrightarrow BAu \in \mathcal{C}^\infty$.

A distribution $u \in \mathcal{D}'(X)$ need not possess a Fourier transform. But if we localize u with a function $\varphi \in \mathcal{C}^\infty_o(X)$ with compact support, then $\widehat{\varphi u}$ is an analytic function which grows at most polynomially (see e.g. [50, Theorem IX.12]). If $supp\,\varphi \cap singsupp\,u = \emptyset$, then $\widehat{\varphi u}$ even decays rapidly (i.e. faster than any inverse power). The next theorem gives a complete characterization of the wavefront set of a distribution via the decay properties of its Fourier transform.

Theorem 2.18 (Theorem 1.8. of [52])

$$(x_o,\xi_o)\notin WF(u) \quad\Leftrightarrow\quad \exists\varphi\in\mathcal{C}_o^\infty,\ \varphi(x_o)\neq 0, \exists \textit{ conic neighborhood } \Gamma \textit{ of } \xi_o \textit{ s.th. } \forall N\in\mathbf{N}: \\ |(\widehat{\varphi u})(\xi)|\le C_N(1+|\xi|)^{-N} \quad \textit{for all } \xi\in\Gamma.$$

Example:
For the δ-distribution in $\mathcal{D}'(\mathbf{R}^n)$ one easily calculates from the criterion of the theorem

$$WF(\delta)=\{(0,\xi);\ \xi\in\mathbf{R}^n\setminus\{0\}\}.$$

The last theorem allows to derive the elegant calculus of wavefront sets which is taken without proofs from [31, section 2.5] in those parts that we need for our purposes. From Theorem 2.18 one again sees that the wavefront set is a local concept, therefore in the following we restrict ourselves to open sets $X\subset\mathbf{R}^n$, but all results are equally valid on manifolds.
First we state a lemma which is a simple consequence of Theorem 2.18, but which we need later on:

Lemma 2.19 *a) Let $u\in\mathcal{D}'(X)$ and $\bar u$ its complex conjugate. Then*

$$WF(\bar u)=\{(x,\xi)\in T^*X;\ (x,-\xi)\in WF(u)\}=:-WF(u). \tag{2.26}$$

*b) Let $v\in\mathcal{D}'(X\times X)$ with $v(\bar f_1,\bar f_2)=\overline{v(f_2,f_1)}$, i.e. $v(x_1,x_2)=\overline{v(x_2,x_1)}$.
Then $WF(v)=-WF(v)$.*

Definition 2.20 *The* **product** *of two distributions u_1,u_2 – if it exists – is defined by convolution of Fourier transforms as the distribution $v\in\mathcal{D}'(X)$ such that $\forall x\in X\ \exists f\in\mathcal{D}(X)$ with $f=1$ near x such that for all $\xi\in\mathbf{R}^n$:*

$$\widehat{f^2v}(\xi)=\frac{1}{(2\pi)^{n/2}}\int_{\mathbf{R}^n}\widehat{fu_1}(\eta)\widehat{fu_2}(\xi-\eta)\ d^n\eta. \tag{2.27}$$

For a detailed discussion of this definition see [50, IX.10], heuristically it means that for a test function $h\in\mathcal{D}(X)$

$$v(h)=\int_X u_1(x)u_2(x)h(x)\ d^nx. \tag{2.28}$$

According to the remark before Theorem 2.18 $\widehat{fu_1}(\eta)$ and $\widehat{fu_2}(\xi-\eta)$ are still polynomially bounded, if η and $\xi-\eta$ are contained in the resp. wavefront sets, but decay rapidly, if not (because of Theorem 2.18). Therefore, for the integral (2.27) to converge (for all ξ) we would expect that it is enough that either η or $-\eta$ is not contained in the resp. wavefront set for all directions η. This is stated in the next theorem.

Theorem 2.21 *Let $u_1,u_2\in\mathcal{D}'(X)$. Suppose that for all $x\in X$:*

$$(x,0)\notin WF(u_1)\oplus WF(u_2):=\{(x,\xi_1+\xi_2);\ (x,\xi_i)\in WF(u_i), i=1,2\}.$$

Then the product u_1u_2 exists and

$$WF(u_1u_2)\subset WF(u_1)\cup WF(u_2)\cup[WF(u_1)\oplus WF(u_2)]. \tag{2.29}$$

Now we consider the restriction of distributions to submanifolds.
Let $\mathcal{M}$ be an n-dimensional manifold and Σ an $(n-1)$-dim. hypersurface (i.e. there exists a $\mathcal{C}^\infty$-imbedding $\varphi : \Sigma \to \mathcal{M}$) with normal bundle

$$N_\varphi := \{(\varphi(y), \xi) \in T^*\mathcal{M};\ y \in \Sigma, \varphi_*(\xi) := {}^t\varphi'(y)\xi = 0\} \tag{2.30}$$

in local coordinates (notation as in Theorem 2.8).
Let $u \in \mathcal{D}'(\mathcal{M})$.
If we could, we would naturally define the restriction $u_\Sigma \in \mathcal{D}'(\Sigma)$ of u to Σ by

$$\begin{aligned} u_\Sigma : f &\mapsto (u \cdot (f\delta_\Sigma))(\mathbf{1}) \quad \text{for } f \in \mathcal{C}_o^\infty(\Sigma) \\ \text{where } f\delta_\Sigma : g &\mapsto \int_\Sigma fg\ d^{n-1}\sigma \quad \text{for } g \in \mathcal{C}_o^\infty(\mathcal{M}), \end{aligned} \tag{2.31}$$

$d^{n-1}\sigma$ is the volume element of Σ, and $\mathbf{1} \in \mathcal{C}_o^\infty(\mathcal{M})$ is a function equal to 1 in a neighborhood of $\{\varphi(y);\ y \in supp\, f\}$.
In (2.31) we must multiply the distributions u and δ_Σ. If Σ is locally given by $t = 0$, then $\delta_\Sigma = \delta(t)$ is the delta-function in the t-variable whose wavefront set is according to the example above

$$\begin{aligned} WF(\delta(t)) &= \{(0, \vec{y}; \lambda, \vec{0}) \in T^*\mathcal{M};\ \vec{y} \in \Sigma, \lambda \neq 0\} \quad \text{or invariantly} \\ WF(\delta_\Sigma) &= \{(x, \xi) \in T^*\mathcal{M};\ x = \varphi(y) \text{ for some } y \in \Sigma, \varphi_*(\xi) = 0, \xi \neq 0\} \\ &= N_\varphi \setminus \{0\}, \end{aligned}$$

hence, by Theorem 2.21, we would expect that formula (2.31) holds for $WF(u) \cap N_\varphi = \emptyset$. This is indeed confirmed by

Theorem 2.22 *Let $\mathcal{M}$, Σ be as above.*
Let $u \in \mathcal{D}'(\mathcal{M})$ with $WF(u) \cap N_\varphi = \emptyset$.
Then the restriction u_Σ of u defined by (2.31) is a well defined distribution in $\mathcal{D}'(\Sigma)$ and

$$WF(u_\Sigma) \subset \varphi_* WF(u) := \{(y, \varphi_*(\xi)) \in T^*\Sigma;\ (\varphi(y), \xi) \in WF(u)\}.$$

The last formula means that the wavefront set becomes projected tangentially onto the surface. The theorem can easily be generalized to arbitrary submanifolds of $\mathcal{M}$.

If we have two properly supported distributions $K_1 \in \mathcal{D}'(X_1 \times X_2)$, $K_2 \in \mathcal{D}'(X_2 \times X_3)$, $X_i \subset \mathbf{R}^{n_i}$, $i = 1, 2, 3$, and if we can compose the corresponding continuous maps to a continuous map

$$K = K_1 \circ K_2 : \mathcal{C}_o^\infty(X_3) \to \mathcal{D}'(X_1),$$

then its kernel distribution is given by

$$K(x_1, x_3) = \int_{X_2} K_1(x_1, x_2) K_2(x_2, x_3)\, dx_2. \tag{2.32}$$

In view of Theorem 2.21 and the fact that $WF(K_2 u) \subset WF_{X_2}(K_2)$ for any $u \in \mathcal{D}(X_3)$ this is well defined if

$$WF'_{X_2}(K_1) \cap WF_{X_2}(K_2) = \emptyset, \tag{2.33}$$

where

$$\begin{aligned}
WF'(K_1) &:= \{(x_1,\xi_1;x_2,-\xi_2) \in T^*X_1 \times T^*X_2;\ (x_1,\xi_1;x_2,\xi_2) \in WF(K_1)\} \\
WF_{X_2}(K_2) &:= \{(x_2,\xi_2) \in T^*X_2;\ (x_2,\xi_2;x_3,0) \in WF(K_2) \text{ for some } x_3 \in X_3\} \\
WF'_{X_2}(K_1) &:= \{(x_2,\xi_2) \in T^*X_2;\ (x_1,0;x_2,\xi_2) \in WF'(K_1) \text{ for some } x_1 \in X_1\},
\end{aligned} \tag{2.34}$$

and we have

Theorem 2.23 *If (2.33) holds for two properly supported distributions $K_1 \in \mathcal{D}'(X_1 \times X_2)$ and $K_2 \in \mathcal{D}'(X_2 \times X_3)$, then the composition (2.32) is a well defined distribution in $\mathcal{D}'(X_1 \times X_3)$ and we have*

$$WF'(K_1 \circ K_2) \subset WF'(K_1) \circ WF'(K_2) \cup (WF_{X_1}(K_1) \times X_3) \cup (X_1 \times WF'_{X_3}(K_2)), \tag{2.35}$$

where X_1 and X_3 are shorthand for $X_1 \times \{0\}$, resp. $X_3 \times \{0\}$, and $WF'(K_1) \circ WF'(K_2)$ means the obvious composition of the two sets.

2.3 The Laplace-Beltrami operator

Now we introduce the Laplace-Beltrami operator on an n-dimensional Riemannian manifold (Σ, h) and cite a result to the effect that certain functions of it (in particular the square-root) are pseudodifferential operators.
If h_{ij} is a positive definite Riemannian metric on a manifold Σ we define the **Laplace-Beltrami operator** by

$$\begin{aligned}
{}^{(n)}\Delta_h u &:= \nabla^i \nabla_i u = h^{ij} \nabla_i \nabla_j u \\
&= \frac{1}{\sqrt{h}} \partial_i \left(\sqrt{h} h^{ij} \partial_j u \right)
\end{aligned} \tag{2.36}$$

for $u \in \mathcal{C}^\infty(\Sigma)$, where h^{ij} is the inverse matrix of h_{ij}, ∇_i is the covariant derivative w.r.t. h_{ij}, h is the determinant of h_{ij} and ∂_i are the partial derivatives in some coordinate system (we simply write Δ when no confusion is possible). It is a positive symmetric operator w.r.t. the natural scalar product $(u_1, u_2) := \int_\Sigma u_1 u_2 \, d^n\sigma$ on $\mathcal{C}_o^\infty(\Sigma)$ ($d^n\sigma := \sqrt{h} d^n x$), since, using Stokes' theorem and the fact that h_{ij} is covariantly constant (i.e. $\nabla_i h_{jk} = 0$)

$$\begin{aligned}
(u_1, \Delta u_2) &= \int_\Sigma u_1 h^{ij} \nabla_i \nabla_j u_2 \, d^n\sigma \\
&= \int_\Sigma h^{ij} (\nabla_i u_1)(\nabla_j u_2) \, d^n\sigma
\end{aligned} \tag{2.37}$$

for $u_1, u_2 \in \mathcal{C}_o^\infty(\Sigma)$. A theorem due to Chernoff [8] shows that Δ (and also all its powers) are essentially selfadjoint on $L^2(\Sigma, d^n\sigma)$ if Σ is a geodesically complete manifold:

Theorem 2.24 (Chernoff [8]) *Let (Σ, h) be a complete n-dimensional Riemannian manifold with Laplace-Beltrami operator ${}^{(n)}\Delta_h$ as given by (2.36) and measure $d^n\sigma$ as in (2.37).*
Then for $\mu \geq 0$ the operator $-{}^{(n)}\Delta_h + \mu^2 : \mathcal{C}_o^\infty(\Sigma) \to L^2(\Sigma, d^n\sigma)$ and all its natural powers are essentially selfadjoint.

Taking the closure $\overline{-\Delta+\mu^2}$ we obtain the unique selfadjoint extension of $-\Delta+\mu^2$ on $L^2(\Sigma, d^n\sigma)$ which we will denote again by $-\Delta+\mu^2$ for simplicity. It is also a positive operator and we can form the square-root $(-\Delta+\mu^2)^{1/2}$ yielding a well defined positive selfadjoint operator on $L^2(\Sigma, d^n\sigma)$, which is even strictly positive (i.e. has no eigenvalue zero) and hence invertible if $\mu > 0$.
On a compact manifold there is a functional calculus for certain pseudodifferential operators (in particular for the square-root of the Laplace-Beltrami operator) due to Seeley [51] and Taylor [52] which we will have the opportunity to use in section 3.3:

Theorem 2.25 *a) Let $A \in L^1_{1,0}(\mathcal{M})$ be an elliptic positive selfadjoint operator on a compact manifold $\mathcal{M}$ with real principal symbol $a(x,\xi)$ which is homogeneous of degree ≤ 1.*
Let $p(\lambda) \in S^m_{\rho,0}(\mathbf{R})$ be a Borel function with $1/2 < \rho \leq 1$.
Then $p(A) \in L^m_{\rho,1-\rho}(\mathcal{M})$ with principal symbol $p(a(x,\xi))$.
b) $A := (-\Delta+\mu^2)^{1/2}$ $(\mu \geq 0)$ on a compact manifold $\mathcal{M}$ is a pseudodifferential operator in $L^1_{1,0}(\mathcal{M})$ with principal symbol $a(x,\xi) = (h^{ij}\xi_i\xi_j)^{1/2}$.

2.4 Parametrices of the Klein-Gordon operator

In this section we consider the Klein-Gordon operator P on a 4-dimensional globally hyperbolic and time-orientable spacetime-manifold $(\mathcal{M}, g)$ and ask for the existence of parametrices of P and their wavefront sets. The following analysis has been carried out by Radzikowski [49] with the methods provided by the general theorems of Duistermaat and Hörmander [16].
Let the Klein-Gordon operator P be given by

$$\begin{aligned} P &:= \Box_g + \mu^2 \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu + \mu^2 \\ &= \frac{1}{\sqrt{|g|}}\partial_\mu\left(\sqrt{|g|}g^{\mu\nu}\partial_\nu \cdot\right) + \mu^2, \end{aligned} \tag{2.38}$$

where $\mu \geq 0$ represents the mass of a scalar field, ∇_μ is the covariant derivative defined by the metric $g_{\mu\nu}$, $g := \det g_{\mu\nu}$, $g^{\mu\nu}$ is the inverse matrix of $g_{\mu\nu}$ and $\partial_\mu = \partial/\partial x^\mu$ the partial derivative in local coordinates.
P is properly supported (by criterion (2.10)) and has the real principal symbol $p(x,\xi) := g^{\mu\nu}(x)\xi_\mu\xi_\nu$, which is homogeneous of degree 2. Put

$$N := p^{-1}(0) \setminus \{0\} = \{(x,\xi) \in T^*\mathcal{M} \setminus \{0\};\ p(x,\xi) = 0\} \tag{2.39}$$

and consider the Hamiltonian vector field (2.25) of p

$$\begin{aligned} H_p &= \sum_{\mu=0}^{3}\left[\frac{\partial p(x,\xi)}{\partial x^\mu}\frac{\partial}{\partial \xi_\mu} - \frac{\partial p(x,\xi)}{\partial \xi_\mu}\frac{\partial}{\partial x^\mu}\right] \\ &= \frac{\partial g^{\kappa\lambda}}{\partial x^\mu}\xi_\kappa\xi_\lambda\frac{\partial}{\partial \xi_\mu} - 2g^{\mu\lambda}\xi_\lambda\frac{\partial}{\partial x^\mu}, \end{aligned} \tag{2.40}$$

which is tangential to N.

Definition 2.26 *The* **bicharacteristic strips** *of P are the integral curves of H_p in N. The* **bicharacteristic curves** *of P are the projections of these strips onto $\mathcal{M}$. The* **bicharacteristic relation** *of P is the set*

$$C := \{(x_1, \xi_1; x_2, \xi_2) \in N \times N;\ (x_1, \xi_1) \textit{ and } (x_2, \xi_2) \textit{ lie on the same bicharacteristic strip}\}.$$

From (2.40) one finds [49] that the bicharacteristic curves of P are the null geodesics of $(\mathcal{M}, g)$ and that

$$C = \{(x_1, \xi_1; x_2, \xi_2) \in N \times N;\ (x_1, \xi_1) \sim (x_2, \xi_2)\}, \tag{2.41}$$

where $(x_1, \xi_1) \sim (x_2, \xi_2)$ means that there is a null geodesic $\gamma : \tau \mapsto x(\tau)$ such that $x(\tau_1) = x_1,\ x(\tau_2) = x_2$ and $\xi_{1\nu} = \dot{x}^\mu(\tau_1) g_{\mu\nu}(x_1),\ \xi_{2\nu} = \dot{x}^\mu(\tau_2) g_{\mu\nu}(x_2)$, i.e. $\xi_1^\mu,\ \xi_2^\mu$ are tangent vectors to the null geodesic γ, and hence parallel transports of each other along γ. (For $x_1 = x_2$ we mean by $(x_1, \xi_1) \sim (x_2, \xi_2)$ that $\xi_1 = \xi_2$.)
Let Δ_N be the diagonal of $N \times N$:

$$\Delta_N := \{(x_1, \xi_1; x_2, \xi_2) \in N \times N;\ x_1 = x_2, \xi_1 = \xi_2\}. \tag{2.42}$$

Then $C \setminus \Delta_N$ decomposes into the open and disjoint sets

$$\begin{aligned} C^+ &:= \{(x_1, \xi_1; x_2, \xi_2) \in N \times N;\ (x_1, \xi_1) \succ (x_2, \xi_2)\} && (2.43)\\ &= \{(x_1, \xi_1; x_2, \xi_2) \in C;\ x_1^0 > x_2^0 \text{ if } \xi_1^0 > 0 \text{ or } x_1^0 < x_2^0 \text{ if } \xi_1^0 < 0\} \\ C^- &:= \{(x_1, \xi_1; x_2, \xi_2) \in N \times N;\ (x_1, \xi_1) \prec (x_2, \xi_2)\} && (2.44)\\ &= \{(x_1, \xi_1; x_2, \xi_2) \in C;\ x_1^0 > x_2^0 \text{ if } \xi_1^0 < 0 \text{ or } x_1^0 < x_2^0 \text{ if } \xi_1^0 > 0\}, \end{aligned}$$

where $(x_1, \xi_1) \prec (\succ) (x_2, \xi_2)$ means $(x_1, \xi_1) \sim (x_2, \xi_2)$ and (x_1, ξ_1) comes after (before) (x_2, ξ_2) w.r.t. the time parameter of the bicharacteristic curve.
$C \setminus \Delta_N = C^+ \dot{\cup} C^-$ is a special case of an orientation of C:

Definition 2.27 *An* **orientation of** C *is a splitting of $C \setminus \Delta_N$ in a disjoint union of open subsets $C \setminus \Delta_N = C^1 \dot{\cup} C^2$ which are inverse relations (i.e. $(x_1, \xi_1; x_2, \xi_2) \in C^1 \Leftrightarrow (x_2, \xi_2; x_1, \xi_1) \in C^2$).*

For the operator P there are exactly 4 orientations, which we want to calculate now:
N has two connected components, namely

$$\begin{aligned} N'_+ &:= \{(x, \xi) \in N;\ \xi^0 > 0\} \\ N'_- &:= \{(x, \xi) \in N;\ \xi^0 < 0\}. \end{aligned} \tag{2.45}$$

We define

$$\begin{aligned} N_1^1 &:= N'_+ \dot{\cup} N'_- = N & N_1^2 &:= \emptyset \\ N_2^1 &:= N'_+ & N_2^2 &:= N'_- \\ N_3^1 &:= N'_- & N_3^2 &:= N'_+ \\ N_4^1 &:= \emptyset & N_4^2 &:= N, \end{aligned}$$

hence $N = N_i^1 \dot{\cup} N_i^2$ for $i = 1, 2, 3, 4$.
Let $B(x, \xi)$ denote the bicharacteristic strip through (x, ξ). Putting

$$C^\pm(x, \xi) := C^\pm \cap (B(x, \xi) \times B(x, \xi))$$

we obtain 4 orientations by

$$
\begin{aligned}
C_i^1 &:= \left(\bigcup_{N_i^1} C^+(x,\xi)\right) \cup \left(\bigcup_{N_i^2} C^-(x,\xi)\right) \\
C_i^2 &:= \left(\bigcup_{N_i^1} C^-(x,\xi)\right) \cup \left(\bigcup_{N_i^2} C^+(x,\xi)\right), \ i = 1,2,3,4.
\end{aligned}
\tag{2.46}
$$

In particular, $C_1^1 = C^+ = C_4^2,\ C_4^1 = C^- = C_1^2,\ C_2^1 = C_3^2,\ C_3^1 = C_2^2$.
It is easy to see that they are inverse relations and that $C \setminus \Delta_N = C_i^1 \dot{\cup} C_i^2$ for $i = 1,2,3,4$. The sets $C_1^1 = C^+,\ C_2^1,\ C_3^1,\ C_4^1 = C^-$ are schematically depicted in Figure 2.1.
The importance of these orientations lies in the fact that they determine uniquely (up to $\mathcal{C}^\infty$) distinguished parametrices of P:

Theorem 2.28 (Theorem 6.5.3. of [16]) *Let P be the Klein-Gordon operator on a globally hyperbolic manifold $(\mathcal{M}, g)$.*
For every orientation $C \setminus \Delta_N = C_i^1 \dot{\cup} C_i^2$, $i = 1,2,3,4$, one can find parametrices E_i^1 and E_i^2 of P with

$$WF'(E_i^1) = \Delta^* \cup C_i^1,\ WF'(E_i^2) = \Delta^* \cup C_i^2$$

where Δ^* is the diagonal in $(T^*\mathcal{M} \setminus \{0\}) \times (T^*\mathcal{M} \setminus \{0\})$. Any right or left parametrix E with $WF'(E)$ contained in $\Delta^* \cup C_i^1$ resp. $\Delta^* \cup C_i^2$ must be equal to E_i^1 resp. E_i^2 modulo a smooth kernel. (WF' was defined in (2.34).)

Since C_2^1 and C_3^1 are nonempty only for x_1 in the future of x_2, resp. x_1 in the past of x_2, the corresponding parametrices E_2^1 and E_3^1 must be (up to $\mathcal{C}^\infty$) the retarded and advanced fundamental solutions $\Delta_R,\ \Delta_A$ of the inhomogeneous Klein-Gordon equation: $E_2^1 = \Delta_R,\ E_3^1 = \Delta_A$. Duistermaat and Hörmander [16, section 6.6] gave E_1^1 and E_4^1 the *names* Feynman and anti-Feynman propagator, Δ_F and $\Delta_{\bar{F}}$, respectively. It was Radzikowski's discovery [49] that these are indeed the (anti-)Feynman-distributions (up to $\mathcal{C}^\infty$) of a Hadamard state of a linear Klein-Gordon quantum field propagating on a curved spacetime. We will take up this remark in section 3.2.
In the next chapter we need the wavefront sets of differences of distinguished parametrices. Therefore we state

Theorem 2.29 *The following holds*
a) $WF'(\Delta_R - \Delta_A) = C$,
b) $WF'(\Delta_R - \Delta_F) = C \cap (N'_- \times N'_-) = \{(x_1,\xi_1;x_2,\xi_2) \in C;\ \xi_1^0 < 0, \xi_2^0 < 0\}$,
c) $WF'(\Delta_F - \Delta_A) = C \cap (N'_+ \times N'_+) = \{(x_1,\xi_1;x_2,\xi_2) \in C;\ \xi_1^0 > 0, \xi_2^0 > 0\}$.

PROOF:
a) From the singular support properties of Δ_R and Δ_A (Theorem 2.28, see Figure 2.1) we see that

$$
\begin{aligned}
\text{for } x_1^0 > x_2^0: \quad WF'(\Delta_R - \Delta_A) &= WF'(\Delta_R) = C_2^1, \\
\text{for } x_1^0 < x_2^0: \quad WF'(\Delta_R - \Delta_A) &= WF'(\Delta_A) = C_3^1.
\end{aligned}
$$

(x_1, ξ_1)

(x_2, ξ_2)

(x_2, ξ_2)

(x_1, ξ_1)

$C_1^1 = WF'(\Delta_F) \setminus \Delta^*$ $\qquad$ $C_2^1 = WF'(\Delta_R) \setminus \Delta^*$

$C_3^1 = WF'(\Delta_A) \setminus \Delta^*$ $\qquad$ $C_4^1 = WF'(\Delta_{\bar{F}}) \setminus \Delta^*$

Figure 2.1: The sets C_1^1, C_2^1, C_3^1, C_4^1 making up the orientations of C and the wavefront sets of distinguished parametrices of the Klein-Gordon operator P.

To determine $WF'(\Delta_R - \Delta_A)$ on the diagonal $x_1 = x_2$ we use that

$$P(\Delta_R - \Delta_A) = 0\,(mod\,\mathcal{C}^\infty) = (\Delta_R - \Delta_A)P,$$

so by Theorem 2.17 the singular directions are parallelly transported along the bicharacteristic curves, hence

$$\Delta_N \subset WF'(\Delta_R - \Delta_A)$$

and therefore

$$WF'(\Delta_R - \Delta_A) = C_2^1 \cup C_3^1 \cup \Delta_N = C.$$

b) Again, by Theorem 2.28 and Figure 2.1 we have that

$$\begin{aligned} \text{for } x_1^0 < x_2^0:\ WF'(\Delta_R - \Delta_F) &= WF'(\Delta_F) = C_1^1|_{x_1^0<x_2^0} = \\ &= \{(x_1,\xi_1;x_2,\xi_2) \in C;\ x_1^0 < x_2^0, \xi_1^0 < 0, \xi_2^0 < 0\}. \end{aligned}$$

To determine $WF'(\Delta_R - \Delta_F)$ for $x_1^0 \geq x_2^0$ we again use the fact that

$$P(\Delta_R - \Delta_F) = 0\,(mod\,\mathcal{C}^\infty) = (\Delta_R - \Delta_F)P,$$

thus, by Theorem 2.17, $WF'(\Delta_R - \Delta_F)|_{x_1^0\geq x_2^0}$ contains the points in $N \times N$ that can be propagated along the bicharacteristic strips from points in $WF'(\Delta_R - \Delta_F)|_{x_1^0<x_2^0}$, hence

$$WF'(\Delta_R - \Delta_F) = \{(x_1,\xi_1;x_2,\xi_2) \in C;\ \xi_1^0 < 0, \xi_2^0 < 0\} = C \cap (N'_- \times N'_-).$$

c) goes as b) □

Corollary 2.30 *It holds*

$$\Delta_R + \Delta_A = \Delta_F + \Delta_{\bar{F}}\,(mod\,\mathcal{C}^\infty).$$

Proof:
Consider $E := \Delta_R + \Delta_A - \Delta_F$.
Since $PE = P\Delta_R + P\Delta_A - P\Delta_F = I\,(mod\,\mathcal{C}^\infty) = EP$, E is a parametrix of P. By the pseudolocal property (Theorem 2.13) of pseudodifferential operators

$$WF'(E) \supset WF'(PE) = WF'(I) = \Delta^*.$$

On the other hand, by (2.20) and Theorem 2.28

$$\begin{aligned} WF'(E) &\subset WF'(\Delta_R) \cup WF'(\Delta_A) \cup WF'(\Delta_F) = \\ &= \Delta^* \cup C_2^1 \cup C_3^1 \cup C_1^1, \end{aligned}$$

but $C_i^1 = \emptyset$ on the diagonal $x_1 = x_2$ for $i = 1,2,3,4$, hence we have on the diagonal $WF'(E)|_{x_1=x_2} = \Delta^*$.
To determine $WF'(E)$ outside the diagonal we use the results of Theorem 2.29:

$$\begin{aligned} \text{for } x_1^0 < x_2^0: \quad WF'(E) &= WF'(\Delta_A - \Delta_F) = C \cap (N'_+ \times N'_+), \\ \text{for } x_1^0 > x_2^0: \quad WF'(E) &= WF'(\Delta_R - \Delta_F) = C \cap (N'_- \times N'_-). \end{aligned}$$

Thus, altogether, $WF'(E) = \Delta^* \cup C_4^1 = WF'(\Delta_{\bar{F}})$, and from the uniqueness of distinguished parametrices (Theorem 2.28) it follows $E = \Delta_{\bar{F}}\,(mod\,\mathcal{C}^\infty)$. □

Chapter 3

Quasifree quantum states of linear scalar fields on curved spacetimes

3.1 The Klein-Gordon field in globally hyperbolic spacetimes

In this work, we are concerned with the quantum theory of the linear Klein-Gordon field in globally hyperbolic spacetimes. We first present the properties of the classical scalar field in order to introduce the phase space that underlies the quantization procedure. Then we construct the Weyl algebra and define the set of quasifree states on it. The material in this section is based on the papers [42, 13, 38]. Here, all function spaces are considered to be spaces of *real* valued functions.
Let us start with the Klein-Gordon equation

$$(\Box_g + \mu^2)\Phi = 0 \tag{3.1}$$

for a scalar field $\Phi : \mathcal{M} \to \mathbf{R}$ on a globally hyperbolic spacetime $(\mathcal{M}, g)$ (see equ. (2.38)). Since (3.1) is a hyperbolic differential equation the Cauchy problem on a globally hyperbolic space is well-posed. As a consequence, there are two unique continuous linear operators

$$\Delta_{R,A} : \mathcal{D}(\mathcal{M}) \to \mathcal{E}(\mathcal{M})$$

with the properties

$$\begin{aligned} (\Box_g + \mu^2)\Delta_{R,A} f = \Delta_{R,A}(\Box_g + \mu^2) f = f \\ supp\,(\Delta_A f) \subset J^-(supp\, f) \\ supp\,(\Delta_R f) \subset J^+(supp\, f) \end{aligned} \tag{3.2}$$

for $f \in \mathcal{D}(\mathcal{M})$. They are called the advanced (Δ_A) and retarded (Δ_R) fundamental solutions of the Klein-Gordon equation (3.1). They are equal (up to smooth kernels) to the distinguished parametrices E_3^1 and E_2^1 of Theorem 2.28. $E := \Delta_R - \Delta_A$ is called the fundamental solution or propagator of (3.1). It has the properties

$$\begin{aligned} (\Box_g + \mu^2) E f = E(\Box_g + \mu^2) f = 0 \\ supp\,(E f) \subset J^+(supp\, f) \cup J^-(supp\, f) \end{aligned} \tag{3.3}$$

for $f \in \mathcal{D}(\mathcal{M})$. We remind ourselves that the wavefront set of E was computed in Theorem 2.29 to be $WF'(E) = C$ with C given in equ. (2.41).
Δ_R, Δ_A and E can be continuously extended to the adjoint operators

$$\Delta_R', \Delta_A', E' : \mathcal{E}'(\mathcal{M}) \to \mathcal{D}'(\mathcal{M})$$

by $\Delta_R' = \Delta_A,\ \Delta_A' = \Delta_R,\ E' = -E$ (this means for the kernel of E: $E(x_1, x_2) = -E(x_2, x_1)$). Let Σ denote a given Cauchy surface of $\mathcal{M}$ with future-directed unit-normalfield n^α. Then there are the restriction operators

$$\begin{aligned} \rho_o :\ & \mathcal{E}(\mathcal{M}) && \to \mathcal{E}(\Sigma) \\ & f && \mapsto f|_\Sigma \\ \rho_1 :\ & \mathcal{E}(\mathcal{M}) && \to \mathcal{E}(\Sigma) \\ & f && \mapsto (n^\alpha \nabla_\alpha f)|_\Sigma, \end{aligned} \tag{3.4}$$

which have adjoints ρ_o', ρ_1' mapping $\mathcal{E}'(\Sigma)$ to $\mathcal{E}'(\mathcal{M})$. Dimock [13] proves the following existence and uniqueness result for the Cauchy problem:

Theorem 3.1 *a) $E\rho_o', E\rho_1'$ restrict to continuous operators from $\mathcal{D}(\Sigma)$ ($\subset \mathcal{E}'(\Sigma)$) to $\mathcal{E}(\mathcal{M})$ ($\subset \mathcal{D}'(\mathcal{M})$) and the unique solution of the Cauchy problem (3.1) with initial data $u_o, u_1 \in \mathcal{D}(\Sigma)$ is given by*

$$u = E\rho_o' u_1 - E\rho_1' u_o. \tag{3.5}$$

b) Furthermore, (3.5) also holds in the sense of distributions, i.e. given $u_o, u_1 \in \mathcal{D}'(\Sigma)$, there exists a unique distribution $u \in \mathcal{D}'(\mathcal{M})$ which is a (weak) solution of (3.1) and has initial data $u_o = \rho_o u, u_1 = \rho_1 u$ (the restrictions in the sense of Theorem 2.22). It is given by

$$u(f) = -u_1(\rho_o E f) + u_o(\rho_1 E f) \tag{3.6}$$

for $f \in \mathcal{D}(\mathcal{M})$.

Applying ρ_o and ρ_1 to the identity (3.5) we immediately obtain:

$$\begin{array}{ll} \rho_o E \rho_0' = 0 & \rho_o E \rho_1' = -1 \\ \rho_1 E \rho_o' = 1 & \rho_1 E \rho_1' = 0 \end{array} \tag{3.7}$$

which reads in a more conventional notation

$$\begin{array}{ll} E(t, \vec{y}_1; t, \vec{y}_2) = 0 & (1 \otimes \mathcal{L}_n) E(t, \vec{y}_1; t, \vec{y}_2) = -\delta(\vec{y}_1, \vec{y}_2) \\ (\mathcal{L}_n \otimes 1) E(t, \vec{y}_1; t, \vec{y}_2) = \delta(\vec{y}_1, \vec{y}_2) & (\mathcal{L}_n \otimes \mathcal{L}_n) E(t, \vec{y}_1; t, \vec{y}_2) = 0 \end{array}$$

in local coordinates, where Σ is given by $t = const.$, $\vec{y} \in \Sigma$ and $\mathcal{L}_n := n^\alpha \nabla_\alpha$ is the Lie derivative in direction n^α. Inserting $u = Ef$ into both sides of equ. (3.5) we get the identity

$$E = E\rho_o' \rho_1 E - E\rho_1' \rho_o E. \tag{3.8}$$

Theorem 3.1 allows us to formulate the classical phase space of the field theory in terms of initial data on a Cauchy surface, we need not consider the solutions themselves. This is of

great advantage for the quantum field theory as we will see soon.
Let Σ be a Cauchy surface for $(\mathcal{M}, g)$ with volume element $d^3\sigma$. Then we define the classical phase space of the Klein-Gordon field as the real linear symplectic space (Γ, σ), where $\Gamma := \mathcal{D}(\Sigma) \oplus \mathcal{D}(\Sigma)$ is the space of initial data with compact support and σ is the symplectic bilinear form

$$\begin{aligned} \sigma : \Gamma \times \Gamma &\rightarrow \mathbf{R} \\ (F_1, F_2) &\mapsto -\int_\Sigma [u_1 p_2 - u_2 p_1]\, d^3\sigma \end{aligned} \tag{3.9}$$

for $F_i := \binom{u_i}{p_i} \in \Gamma, i = 1, 2$.
(3.9) is independent of the choice of Cauchy surface: If Σ_1 and Σ_2 are two Cauchy surfaces (enclosing the volume $V \subset \mathcal{M}$) and Φ_1, Φ_2 the solutions of (3.1) to the initial data F_1, F_2 on Σ_1 (with compact supports) then we can write (3.9) as

$$\begin{aligned} -\sigma(\Phi_1, \Phi_2) &= \int_{\Sigma_1} [\Phi_1 \nabla_\alpha \Phi_2 - \Phi_2 \nabla_\alpha \Phi_1] n^\alpha \, d^3\sigma \\ &\equiv \int_{\Sigma_1} j_\alpha n^\alpha \, d^3\sigma \\ &= \int_V (\nabla^\alpha j_\alpha)\, d^4\mu + \int_{\Sigma_2} j_\alpha n^\alpha \, d^3\sigma \\ &= \int_{\Sigma_2} j_\alpha n^\alpha \, d^3\sigma \\ &\equiv \int_{\Sigma_2} [\Phi_1 \nabla_\alpha \Phi_2 - \Phi_2 \nabla_\alpha \Phi_1] n^\alpha \, d^3\sigma \end{aligned}$$

since j_α is the conserved current $(\nabla^\alpha j_\alpha = 0)$ of the Klein-Gordon field.

Now, to the symplectic space (Γ, σ) there is associated (uniquely up to unitary equivalence) a Weyl algebra $\mathcal{A}[\Gamma, \sigma]$, which is a simple C^*-algebra generated by the elements $W(F)$, $F \in \Gamma$, that satisfy

$$\begin{aligned} &W(F)^* = W(F)^{-1} = W(-F) \quad \text{(unitarity)} \\ &W(F_1)W(F_2) = e^{-\frac{i}{2}\sigma(F_1, F_2)} W(F_1 + F_2) \quad \text{(Weyl relations)} \end{aligned} \tag{3.10}$$

for all $F_1, F_2 \in \Gamma$. We can think of the elements $W(F)$ as the exponentiated field operators $e^{i\hat{\Phi}(f)}$, smeared with testfunctions $f \in \mathcal{D}(\mathcal{M})$, where $F = \binom{\rho_o Ef}{\rho_1 Ef}$. (3.10) then corresponds to the canonical commutation relations.
A local algebra $\mathcal{A}(\mathcal{O})$ ($\mathcal{O}$ an open bounded subset of $\mathcal{M}$) is the C^*-algebra generated by the elements $W(\rho_o Ef, \rho_1 Ef)$ with $supp\, f \subset \mathcal{O}$. It is the algebra of quantum observables measurable in the spacetime region $\mathcal{O}$. Then $\mathcal{A}[\Gamma, \sigma] = \overline{\bigcup_{\mathcal{O}} \mathcal{A}(\mathcal{O})}^{C^*}$.
Dimock [13] has shown that $\mathcal{O} \mapsto \mathcal{A}(\mathcal{O})$ is a net of local observable algebras in the sense of Haag and Kastler [26], i.e. it satisfies
i) $\mathcal{O}_1 \subset \mathcal{O}_2 \Rightarrow \mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$ (isotony).
ii) $\mathcal{O}_1$ spacelike separated from $\mathcal{O}_2 \Rightarrow [\mathcal{A}(\mathcal{O}_1), \mathcal{A}(\mathcal{O}_2)] = \{0\}$ (locality).
iii) There is a faithful irreducible representation of $\mathcal{A}$ (primitivity).
iv) $\mathcal{O}_1 \subset D(\mathcal{O}_2) \Rightarrow \mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$.

v) For any isometry $\kappa : (\mathcal{M}, g) \to (\mathcal{M}, g)$ there is an isomorphism $\alpha_\kappa : \mathcal{A} \to \mathcal{A}$ such that $\alpha_\kappa[\mathcal{A}(\mathcal{O})] = \mathcal{A}(\kappa(\mathcal{O}))$ and $\alpha_{\kappa_1} \circ \alpha_{\kappa_2} = \alpha_{\kappa_1 \circ \kappa_2}$ (covariance).

The states on an observable algebra $\mathcal{A}$ are the linear functionals $\omega : \mathcal{A} \to \mathbf{C}$ satisfying $\omega(\mathbf{1}) = 1$ (normalization) and $\omega(A^* A) \geq 0 \; \forall A \in \mathcal{A}$ (positivity). The set of states on our Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ is by far too large to be tractable in a concrete way. Therefore, for linear systems, one usually restricts oneself to the quasifree states, all of whose truncated n-point functions vanish for $n \neq 2$:

Definition 3.2 *Let $\mu : \Gamma \times \Gamma \to \mathbf{R}$ be a real scalar product satisfying*

$$\frac{1}{4}|\sigma(F_1, F_2)|^2 \leq \mu(F_1, F_1)\mu(F_2, F_2) \tag{3.11}$$

for all $F_1, F_2 \in \Gamma$. Then the **quasifree state** *ω_μ associated with μ is given by*

$$\omega_\mu(W(F)) = e^{-\frac{1}{2}\mu(F,F)}. \tag{3.12}$$

If ω_μ is pure it is called a **Fock state***.*

The connection between this algebraic notion of a quasifree state and the usual notion of "vacuum state" in a Hilbert space is established by the following theorem which we cite from [38]:

Theorem 3.3 *Let ω_μ be a quasifree state on $\mathcal{A}[\Gamma, \sigma]$.*

a) Then there exists a **one-particle Hilbertspace structure***, i.e. a Hilbert space $\mathcal{H}$ and a real-linear map $k : \Gamma \to \mathcal{H}$ such that*
i) $k\Gamma + ik\Gamma$ is dense in $\mathcal{H}$,
ii) $\mu(F_1, F_2) = \mathrm{Re}\langle kF_1, kF_2\rangle_{\mathcal{H}} \; \forall F_1, F_2 \in \Gamma$,
iii) $\sigma(F_1, F_2) = 2\mathrm{Im}\langle kF_1, kF_2\rangle_{\mathcal{H}} \; \forall F_1, F_2 \in \Gamma$.
Moreover, the pair $(k, \mathcal{H})$ is uniquely determined up to unitary equivalence.
It holds: ω_μ is pure $\Leftrightarrow$ $k(\Gamma)$ is dense in $\mathcal{H}$.

b) The GNS-triple $(\mathcal{H}_{\omega_\mu}, \pi_{\omega_\mu}, \Omega_{\omega_\mu})$ of the state ω_μ can be represented as $(\mathcal{F}^s(\mathcal{H}), \rho_\mu, \Omega^{\mathcal{F}})$, where
i) $\mathcal{F}^s(\mathcal{H})$ is the symmetric Fock space over the one-particle Hilbert space $\mathcal{H}$,
ii) $\rho_\mu[W(F)] = \exp\{-i\overline{[a^*(kF) + a(kF)]}\}$, where a^* and a are the standard creation and annihilation operators on $\mathcal{F}^s(\mathcal{H})$ satisfying

$$[a(u), a^*(v)] = \langle u, v\rangle_{\mathcal{H}} \text{ and } a(u)\Omega^{\mathcal{F}} = 0$$

for $u, v \in \mathcal{H}$ (the bar denotes the closure of the operator).
iii) $\Omega^{\mathcal{F}} := \mathbf{1} \oplus \mathbf{0} \oplus \mathbf{0} \oplus \ldots$ is the (cyclic) Fock vacuum.
It holds: ω_μ is pure $\Leftrightarrow$ ρ_μ is irreducible.

Thus, ω_μ can also be represented as $\omega_\mu(W(F)) = \exp\{-\frac{1}{2}||kF||^2_{\mathcal{H}}\}$ (in case a)) or $\omega_\mu(W(F)) = \langle\Omega^{\mathcal{F}}, \rho_\mu(F)\Omega^{\mathcal{F}}\rangle$ (in case b)). $\hat{\Phi}(F) := a^*(kF) + a(kF)$ is the usual field operator on $\mathcal{F}^s(\mathcal{H})$ and we can determine the ("symplectically smeared") two-point function as

$$\begin{aligned}\lambda^{(2)}(F_1,F_2) &= \langle \Omega^{\mathcal{F}}, \hat{\Phi}(F_1)\hat{\Phi}(F_2)\Omega^{\mathcal{F}}\rangle \\ &= \langle kF_1, kF_2\rangle_{\mathcal{H}} \\ &= \mu(F_1,F_2) + \frac{i}{2}\sigma(F_1,F_2)\end{aligned} \tag{3.13}$$

for $F_1, F_2 \in \Gamma$, resp. the "four-smeared" (Wightman) two-point distribution as

$$\Lambda^{(2)}(f_1,f_2) = \lambda^{(2)}\left(\begin{pmatrix}\rho_o E f_1\\ \rho_1 E f_1\end{pmatrix}, \begin{pmatrix}\rho_o E f_2\\ \rho_1 E f_2\end{pmatrix}\right) \tag{3.14}$$

for $f_1, f_2 \in \mathcal{D}(\mathcal{M})$. The fact that the antisymmetric (= imaginary) part of $\lambda^{(2)}$ is the symplectic form σ implies for $\Lambda^{(2)}$:

$$\begin{aligned}\mathrm{Im}\Lambda^{(2)}(f_1,f_2) &= -\frac{1}{2}\int_\Sigma [f_1 E'\rho_o'\rho_1 E f_2 - f_1 E'\rho_1'\rho_o E f_2]\, d^3\sigma \\ &= \frac{1}{2}\langle f_1, E f_2\rangle\end{aligned} \tag{3.15}$$

by equ. (3.8). All the other n-point functions can also be calculated, one finds that they vanish if n is odd and that the n-point functions for n even are sums of products of two-point functions. We want to stress that the restriction to quasifree states is a priori not physically motivated but by the fact that they are exclusively determined by their two-point function and therefore easily tractable. Nevertheless, one gets a large class of states including e.g. the usual vacuum state on stationary spacetimes or the so-called "frequency splitting vacua" obtained by mode-decomposition of the field operators (see e.g. [5]), but it also contains all sorts of unphysical states. Therefore, as was discussed in the introduction, we have to impose certain selection criteria even on this restricted class of states. This will be done in sections 3.2 and 3.4 where we introduce quasifree Hadamard states and adiabatic vacuum states and show that they in fact select the same local folium of states. Since the folium of a quasifree state also contains states that are not quasifree one can in principle get statements about a larger class of states than merely the quasifree ones. Recently, Kay [37] considered also states that allow for a non-vanishing one-point function.

A curved spacetime does in general not possess any isometries, hence property v) above of the net of local algebras is in general empty. But there is the important class of spacetimes possessing a timelike Killing vectorfield that deserves further attention.
Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold, foliated into spacelike Cauchy surfaces $\mathcal{M} = \mathbf{R}\times\Sigma$, $\Sigma_t = \{t\}\times\Sigma$, and possessing a one-parameter group of isometries $\tau_t : \mathcal{M}\to\mathcal{M}, t\in\mathbf{R}$, such that $\tau_t(\Sigma_{t_o}) = \Sigma_{t_o+t}$. Define $\mathcal{T}(t) : \Gamma\to\Gamma$ by

$$\mathcal{T}(t)F_{t_o} := F_{t_o+t}$$

where F_{t_o}, F_{t_o+t} are the Cauchy data of a solution of (3.1) taken on Cauchy surfaces Σ_{t_o} resp. Σ_{t_o+t}. Since the symplectic form σ is invariant under the action of $\mathcal{T}(t)$ and since $\mathcal{T}(t)\mathcal{T}(s) = \mathcal{T}(t+s)\ \forall t,s\in\mathbf{R}$, $\mathcal{T}(t)$ is a one-parameter group of symplectic transformations (also called Bogoliubov transformations). It gives rise to a group of automorphisms $\alpha(t), t \in \mathbf{R}$, (Bogoliubov automorphisms) on the algebra $\mathcal{A}$ via

$$\alpha(t)W(F) = W(\mathcal{T}(t)F).$$

In this case, there exists a preferred class of states on $\mathcal{A}$, namely those invariant under $\alpha(t)$. A quasifree state ω_μ will be invariant under this symmetry if and only if

$$\mu(\mathcal{T}(t)F_1, \mathcal{T}(t)F_2) = \mu(F_1, F_2) \; \forall t \in \mathbf{R} \; \forall F_1, F_2 \in \Gamma.$$

The automorphism group $\alpha(t)$ can be unitarily implemented in the one-particle Hilbertspace structure $(k, \mathcal{H})$ of an invariant state ω_μ, i.e. there exists a unitary group $U(t), t \in \mathbf{R}$, on $\mathcal{H}$ satisfying

$$\begin{aligned} U(t)k &= k\mathcal{T}(t) \\ U(t)U(s) &= U(t+s). \end{aligned} \tag{3.16}$$

(This follows easily from the uniqueness statement of Theorem 3.3a).) If $U(t)$ is strongly continuous it takes the form $U(t) = e^{-iht}$ for some self-adjoint operator h on $\mathcal{H}$.
We are now ready to define two particularly important classes of states (we follow [35]):

Definition 3.4 *Let the phase space $(\Gamma, \sigma, \mathcal{T}(t))$ be given.*

a) A quasifree **ground state** *is a quasifree state over $\mathcal{A}[\Gamma, \sigma]$ with one-particle Hilbertspace structure $(k, \mathcal{H})$ and a strongly continuous unitary group $U(t) = e^{-iht}$ (satisfying (3.16)) such that h is a positive operator (the "one-particle Hamiltonian").*

b) A quasifree **KMS-state** *is a quasifree state over $\mathcal{A}[\Gamma, \sigma]$ with one-particle Hilbertspace structure $(k^\beta, \tilde{\mathcal{H}})$ and a strongly continuous unitary group $U(t) = e^{-i\tilde{h}t}$ (satisfying (3.16)) such that the "one-particle KMS-condition" is satisfied, namely $\forall u, v \in k^\beta\Gamma \; \forall t \in \mathbf{R}$:*

$$\langle e^{-it\tilde{h}}u, v\rangle_{\tilde{\mathcal{H}}} = \langle e^{-\frac{\beta\tilde{h}}{2}}v, e^{-it\tilde{h}}e^{-\frac{\beta\tilde{h}}{2}}u\rangle_{\tilde{\mathcal{H}}}. \tag{3.17}$$

Although the definition of ground- and KMS-states can be given in a very general context (see e.g. [24]), we have restricted ourselves to the case of quasifree states on the Weyl algebra since this is the only situation we consider here. The physical interpretation of these stationary states is the following: The ground state is the state of lowest energy of the theory, it is closest to what one would call the vacuum state in Minkowski space. It fulfills the spectrum condition in that h has positive spectrum. A KMS-state is a thermodynamic equilibrium state of the theory at temperature $1/\beta$. The KMS-condition (3.17) is the generalization of the Gibbs equilibrium condition to infinite systems. It was introduced into quantum field theory by Haag, Hugenholtz and Winnink [25]. We will present an explicit construction of ground- and KMS-states on ultrastatic spacetimes in section 3.3.

3.2 Hadamard states

Now we introduce the notion of Hadamard states. Following Kay and Wald [38] we state the original definition of Hadamard states and some of its consequences. Then we introduce Radzikowski's local characterization of Hadamard states [49] and discuss its relevance for quantum field theory on curved spacetimes. First we need some preparatory definitions.

Definition 3.5 *Let Σ be a spacelike Cauchy surface of $(\mathcal{M}, g)$.*
A **causal normal neighborhood** *N of Σ is an open neighborhood of Σ in $\mathcal{M}$ such that Σ is a Cauchy surface for N and such that for all $x_1, x_2 \in N$ with $x_1 \in J^+(x_2)$ there exists a convex normal neighborhood which contains $J^-(x_1) \cap J^+(x_2)$. (As a consequence, the squared geodesic distance $\sigma(x_1, x_2)$ is then well defined and smooth for all causally related pairs of points in N).*

Lemma 3.6 (Lemma 2.2 of [38]) *For each spacelike Cauchy surface Σ there exists a causal normal neighborhood N.*

We choose a preferred time orientation on $(\mathcal{M}, g)$ and a smooth global time function $T : \mathcal{M} \to \mathbf{R}$ which increases towards the future. Let $\mathcal{O} \subset \mathcal{M} \times \mathcal{M}$ be an open neighborhood of the set of causally related points (x_1, x_2) such that $J^+(x_1) \cap J^-(x_2)$ and $J^-(x_1) \cap J^+(x_2)$ are contained within a convex normal neighborhood and $\mathcal{O}'$ an open neighborhood in $N \times N$ of the set of causally related points such that $\overline{\mathcal{O}'} \subset \mathcal{O}$.
Within $\mathcal{O}$ the squared geodesic distance $\sigma(x_1, x_2)$ is well defined and we define for each $n \in \mathbf{N}$ a real function $v^{(n)} \in \mathcal{C}^\infty(\mathcal{O})$ as the power series

$$v^{(n)}(x_1, x_2) := \sum_{m=0}^{n} v_m(x_1, x_2)\sigma^m \tag{3.18}$$

where the v_m are uniquely determined by the Hadamard recursion relations (see [12]); note that the v_m are solely determined by the mass μ of the Klein-Gordon field and the metric g of the spacetime).
Let $\chi \in \mathcal{C}^\infty(N \times N)$ be a function with the property that

$$\chi(x_1, x_2) = \begin{cases} 0, & \text{for } (x_1, x_2) \notin \mathcal{O} \\ 1, & \text{for } (x_1, x_2) \in \mathcal{O}'. \end{cases}$$

For each $n \in \mathbf{N}$ and $\epsilon > 0$ we define in $\mathcal{O}$ the (complex valued) function

$$G_\epsilon^{T,n}(x_1, x_2) := \frac{1}{(2\pi)^2}\left(\frac{\Delta(x_1, x_2)^{1/2}}{\sigma + 2i\epsilon(T(x_1) - T(x_2)) + \epsilon^2} + v^{(n)}(x_1, x_2)\ln(\sigma + 2i\epsilon(T(x_1) - T(x_2)) + \epsilon^2)\right), \tag{3.19}$$

where Δ is the van Vleck-Morette determinant [12] and the branch-cut for the logarithm is taken to lie along the negative real axis. Now we are ready to define:

Definition 3.7 *Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold, Σ a Cauchy surface of $\mathcal{M}$, N a causal normal neighborhood of Σ and $\chi, T, G_\epsilon^{T,n}$ as above.*
Then we call a quasifree state ω of the Weyl-algebra $\mathcal{A}$ of the Klein-Gordon field on $(\mathcal{M}, g)$ a

(global) Hadamard state *if its two-point distribution* $\Lambda^{(2)}$ *is such that there exists a sequence of functions* $H^n \in \mathcal{C}^n(N \times N)$ *such that for all* $f_1, f_2 \in \mathcal{C}_o^\infty(N)$ *and all* $n \in \mathbf{N}$ *we have*

$$\Lambda^{(2)}(f_1, f_2) = \lim_{\epsilon\to 0} \int_{N\times N} \Lambda_\epsilon^{T,n}(x_1, x_2) f_1(x_1) f_2(x_2)\, d^4\mu(x_1) d^4\mu(x_2), \tag{3.20}$$

$$\text{where } \Lambda_\epsilon^{T,n}(x_1, x_2) := \chi(x_1, x_2) G_\epsilon^{T,n}(x_1, x_2) + H^n(x_1, x_2). \tag{3.21}$$

Note that χ was chosen to be zero where $G_\epsilon^{T,n}$ was not defined, so $\Lambda_\epsilon^{T,n}$ is well defined throughout $N \times N$. Kay and Wald [38] show that the definition is actually independent of the choice of N, χ and T. In [23] it was proved that the Hadamard property of a state is preserved under Cauchy evolution, i.e. if $\Lambda^{(2)}$ is of the Hadamard form in a causal normal neighborhood N of some Cauchy surface Σ, then it is of Hadamard form in some causal normal neighborhood N' of any other Cauchy surface Σ'. This implies in particular, that the Definition 3.7 above is independent of the choice of Σ, too.
In [22] it is established that in any globally hyperbolic spacetime there is always a class of quantum states, forming a dense subspace of a Hilbert space, whose two-point functions have the Hadamard singularity structure (3.20).
The essential ingredient in the Definition 3.7 is the specification of the singularity structure (3.19) of the two-point distribution (3.20). It is the same for all Hadamard states, whereas the smooth part H^n in (3.21) depends on the respective state. This was the original motivation for the consideration of Hadamard states because it allows for the renormalization of the energy-momentum tensor. For a Klein-Gordon field Φ the energy-momentum tensor is given by

$$T_{\mu\nu}[\Phi] = (\nabla_\mu \Phi)(\nabla_\nu \Phi) - \frac{1}{2} g_{\mu\nu} (\nabla_\kappa \Phi \nabla^\kappa \Phi - \mu^2 \Phi^2). \tag{3.22}$$

In order that the semiclassical Einstein equations

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi \left\langle \hat{T}_{\mu\nu}(x) \right\rangle_\omega \tag{3.23}$$

make sense, one must define the expectation value of the energy-momentum operator $\hat{T}_{\mu\nu}$ of the quantum field Φ in the state ω at a spacetime point x. One procedure which has been studied in great detail is the point-splitting renormalization [10, 2, 1, 56, 57]. In this approach one regards initially $\langle \hat{T}_{\mu\nu}(x, x')\rangle_\omega$ as a two-point distribution (note that $T_{\mu\nu}$ is quadratic in Φ resp. its derivatives), which, however, behaves singular in the "coincidence limit" $x \to x'$. But if we admit only states ω whose two-point distributions have the same singularity structure, as is the case for Hadamard states, then we can subtract from $\langle \hat{T}_{\mu\nu}(x, x')\rangle_\omega$ another distribution with this singularity structure and *define* the renormalized value of $\langle \hat{T}_{\mu\nu}(x)\rangle_\omega$ as the coincidence limit of this difference. Wald [56, 57] formulated a set of axioms that a physically reasonable $\langle \hat{T}_{\mu\nu}\rangle$ should satisfy and showed that for Hadamard states the point-splitting prescription gives a result consistent with these axioms. However, there remains an ambiguity of adding local curvature terms. (For a discussion of this non-uniqueness see [21].) Recently, a different renormalization scheme has been investigated by Köhler [40]. He utilizes the cancellation of singularities in $\langle \hat{T}_{\mu\nu}\rangle$ that occur between two scalar fields and one Dirac field in Hadamard states. This technique yields results consistent with the point-splitting renormalization, but works only on vacuum spacetimes. Thus, although it seems that the last word on $\langle \hat{T}_{\mu\nu}\rangle$ has not

yet been said, it is clear that the Hadamard states play an important rôle in its definition.
In [55], Verch showed that any two Hadamard states for the Klein-Gordon field on a globally hyperbolic manifold are locally quasiequivalent. For a more restricted class of spacetimes, the ultrastatic ones (see Definition 3.11 below), he proved that the local von Neumann algebras are type III_1-factors and that the Reeh-Schlieder property holds [54]. All these facts strongly suggest that the local quasiequivalence class of states generated by the Hadamard states is a good candidate for the set of physical states of scalar quantum fields on globally hyperbolic manifolds.
However, the Hadamard states – as they were defined above – have also some severe drawbacks. Firstly, the Definition 3.7 is tailored for free fields. Note that the $v^{(n)}$ in (3.19) are constructed in such a way that the two-point function (3.20) is a distributional bi-solution of the Klein-Gordon equation. It is not clear in this formulation how one could obtain a generalization to nonlinear, interacting fields.
Secondly, the Definition 3.7 is a global definition in the sense that the singularity structure has to be specified for spacetime points x_1, x_2 ranging over a neighborhood of the whole Cauchy surface; it states that there are no singularities at points $(x_1, x_2) \in N \times N$ s.th. x_1 is spacelike separated from x_2. Our experience with local quantum physics and the very concept of general relativity suggest that the physical information of a theory is encoded locally, i.e. in an arbitrarily small neighborhood of each spacetime point. This was pointed out by Fredenhagen and Haag [17] and led Kay [36] to conjecture that if already a local version of Definition 3.7 is satisfied for a state then its two-point distribution should not have singularities at spacelike separated points. Let us give a precise definition of this "local version":

Definition 3.8 *Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold.*
A two-point distribution $\Lambda^{(2)} \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ is said to be **locally Hadamard** *if for each $x \in \mathcal{M}$ there is an open neighborhood U_x of x s.th. for each $n \in \mathbf{N}$ $\Lambda^{(2)}|_{U_x \times U_x}$ coincides with $(\lim_{\epsilon\to 0} \Lambda_\epsilon^{T,n})|_{U_x \times U_x}$ (equ. (3.21)) of a global Hadamard state when the Cauchy surface Σ, causal normal neighborhood N and U_x are chosen such that $U_x \subset N$.*

That Kay's conjecture is indeed true was recently shown by Radzikowski [49] in a very remarkable work. He realized that the local information on the Hadamard property is encoded in the wavefront set of the two-point distribution and proved the following important theorem:

Theorem 3.9 (Theorem 2.6 of [49], see also [39]) *A quasifree state of a Klein-Gordon quantum field on a globally hyperbolic spacetime is a (global) Hadamard state if and only if its two-point distribution $\Lambda^{(2)}$ possesses the following wavefront set:*

$$WF(\Lambda^{(2)}) = \{(x_1, \xi_1; x_2, -\xi_2) \in T^*(\mathcal{M} \times \mathcal{M}) \setminus \{0\};\ (x_1, \xi_1) \sim (x_2, \xi_2), \xi_1^0 \geq 0\}. \tag{3.24}$$

The notation was introduced in section 2.4: $(x_1, \xi_1) \sim (x_2, \xi_2)$ means that x_1 and x_2 can be connected by a null geodesic γ such that ξ_1^μ is tangential to γ at x_1, and ξ_2^μ is the parallel transport of ξ_1^μ along γ at x_2. On the diagonal $x_1 = x_2$ $(x_1, \xi_1) \sim (x_2, \xi_2)$ means that $\xi_1 = \xi_2$, $\xi_1^2 = 0$. The wavefront set (3.24) is schematically depicted in Figure 3.1.

Note that $\Lambda^{(2)}$ is a solution of the Klein-Gordon equation in both arguments and that therefore $WF(\Lambda^{(2)}) \subset N \times N$ (N was defined in equ. (2.39)). Hence, the essential physical

(x_1, ξ_1)

(x_2, ξ_2) $\qquad \cup \qquad$ $(x, \xi; x, \xi)$

(x_1, ξ_1)

Figure 3.1: The wavefront set $WF'(\Lambda^{(2)})$ of an Hadamard two-point distribution $\Lambda^{(2)}$.

content of Theorem 3.9 is that singularities only occur if x_1 and x_2 are lightlike connected and that the singularities only have *positive* frequencies. This is the remnant of the spectrum condition of quantum field theory on Minkowski space. In fact, already in [50] it was shown that the vacuum state of a linear scalar quantum field on Minkowski space fulfills (3.24). This was used in [49] and [39] to prove Theorem 3.9.
From Theorem 3.9 it easily follows [49] that the **Feynman propagator**

$$E_F := i\Lambda^{(2)} + \Delta_A \tag{3.25}$$

of a Hadamard state is equal (up to $\mathcal{C}^\infty$) to the distinguished parametrix $\Delta_F \equiv E_1^1$ of Theorem 2.28. With the new characterization of Hadamard states by their wavefront set at his disposal Radzikowski was able to prove the following "**local-to-global-singularity theorem**":

Theorem 3.10 (Theorem 3.3 of [49]) *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime. Any quasifree state of a Klein-Gordon quantum field on $(\mathcal{M}, g)$ whose two-point distribution is locally Hadamard (Definition 3.8) is a global Hadamard state (Definition 3.7).*

This says that local physical information leads uniquely to global physical information and verifies Kay's conjecture.
Since the wavefront set is a covariant and locally defined object on a manifold (properties 1) and 2) of section 2.2) the characterization of Hadamard states by the wavefront set of their two-point distributions promises to be a very useful tool for quantum field theory on curved spacetime, and from now on we will take Theorem 3.9 as a *definition* of Hadamard state.
A first important observation is that the concept of the wavefront set is no longer tied to a certain linear field equation. Therefore (3.24) is a possible starting point for a characterization of the physical states of an arbitrary interacting quantum field. The idea is of course to specify the wavefront set of all the n-point Wightman functions of the quantum fields. Radzikowski [49] gave a first proposal of such a wavefront set spectrum condition, as he called it. In [7] it

is argued that this condition is not consistent and a new one is suggested which is shown to be satisfied for Wick ordered products of fields. In [39] the Theorems 2.21 and 3.9 were used to define the product of two scalar fields in an Hadamard product state as a new Wightman field on manifolds. In this case there may also appear lightlike singularities, but at any rate no spacelike ones.
These first results indicate that the wavefront set is the relevant mathematical object in order to investigate general properties of quantum field theory on curved spacetimes.

3.3 Ultrastatic ground- and KMS-states

In this section we want to show that wavefront sets and pseudodifferential operators also are a very useful tool for analysing concrete physical states for linear fields on certain spacetime models. Up to now there have not many states been constructed which are known to be Hadamard states, but a great many more which have not been characterized as physical or not in such a way. Among the best investigated examples are states for Klein-Gordon fields on ultrastatic spacetimes, the Schwarzschild (resp. Kruskal-) spacetime and the Robertson-Walker spacetimes. On Robertson-Walker spacetimes there exists the large class of "adiabatic vacua" which we will investigate in detail in the next section. On the Schwarzschild spacetime we explicitly know the groundstate w.r.t. the timelike Killing field (the "Boulware vacuum" [6, 34]), the thermodynamic equilibrium states (KMS-states [34]) and the Unruh state [53, 15, 14], which describes the outflow of thermal radiation from an eternal black hole. These are stationary quasifree states. Kay and Wald [38] showed that on spacetimes with bifurcate Killing horizons (e.g. the Kruskal extension of the Schwarzschild metric) there can be at most one stationary Hadamard state. This is the KMS-state at the Hawking temperature $1/8\pi M$, where M is the mass of the black hole (the so-called Hartle-Hawking state [28]). This result indicates that it is the Hadamard condition which is responsible for singling out the states that describe the thermal radiation of a star collapsing to a black hole, which was discovered by Hawking in his famous paper [29]. And indeed, in [18] it is derived that in the gravitational collapse of a spherically symmetric star all quantum states which have the Hadamard property (in fact a somewhat weaker scaling condition) at the intersection of the surface of the star and the Schwarzschild radius are seen by asymptotic detectors (at large radial distances and late times) as a thermal radiation (modified by a gravitational barrier penetration effect) at the Hawking temperature $1/8\pi M$. For a rotating black hole (Kerr metric) a similar computation has been performed in [30]. On ultrastatic spacetimes it has been proven [22, 58] that the ground state is a Hadamard state. We will now give a new proof of this result. On the one hand, our proof is much more transparent than that of [22, 58] since we use the techniques of wavefront sets and pseudodifferential operators, on the other hand it easily extends to the ultrastatic KMS-states and also gives the essential ideas that are used to prove the Hadamard property of the adiabatic vacua in the next section.

Definition 3.11 *A spacetime $(\mathcal{M}, g)$ is* **ultrastatic** *if it possesses a timelike Killing field t^μ which is hypersurface-orthogonal and obeys $g_{\mu\nu}t^\mu t^\nu = 1$.*

This is a slight specialization of a static spacetime where one dispenses with the last condition. A static spacetime possesses a global foliation $\mathcal{M} = \mathbf{R} \times \Sigma$ into spacelike hypersurfaces $\Sigma_t = \{t\} \times \Sigma, t \in \mathbf{R}$. If $\{x^i, i = 1,2,3\}$ is a local coordinate system for Σ the static metric can be written as

$$ds^2 = \alpha(\vec{x})^2 dt^2 - h_{ij}(\vec{x}) dx^i dx^j, \tag{3.26}$$

where $\alpha \in \mathcal{C}^\infty(\Sigma)$ is the "lapse function" and h_{ij} a Riemannian metric on Σ (both of them independent of t), and $t^\mu = (\partial/\partial t)^\mu$ is the timelike Killing field orthogonal to Σ_t.
The ultrastatic case is now the special situation where $\alpha \equiv 1$, i.e. the metric is

$$ds^2 = dt^2 - h_{ij}(\vec{x}) dx^i dx^j \tag{3.27}$$

in a local coordinate system. In this case we have:

Lemma 3.12 (see [32]) *Let $(\mathcal{M}, g)$ be an ultrastatic spacetime. Then the following are equivalent:*
1.) $(\mathcal{M}, g)$ is globally hyperbolic.
2.) Σ_t is a Cauchy surface for each t.
3.) (Σ, h) is geodesically complete.

Thus, by Theorem 2.24, for a globally hyperbolic ultrastatic spacetime we can define $A := \overline{-^{(3)}\Delta_h + \mu^2}$ as a positive selfadjoint operator on $L^2_{\mathbf{C}}(\Sigma, d^3\sigma)$ which is invertible for $\mu > 0$, and likewise all its powers ($^{(3)}\Delta_h$ denotes the Laplace-Beltrami operator on Σ w.r.t. the metric h_{ij}, the bar denotes the closure of the operator). In this situation, we can define the "canonical vacuum state" on the Weyl algebra of the Klein-Gordon field in the following way [32]:
Let (Γ, σ) denote the real symplectic space of initial data $\Gamma := \mathcal{C}^\infty_o(\Sigma_t) \oplus \mathcal{C}^\infty_o(\Sigma_t)$ on a Cauchy surface Σ_t with the symplectic form

$$\sigma(F_1, F_2) := -\int_{\Sigma_t} d^3\sigma \, [f_1 p_2 - p_1 f_2], \tag{3.28}$$

where $d^3\sigma := \sqrt{h}\, d^3x, \; h := \det h_{ij}, \; F_i := \binom{f_i}{p_i} \in \Gamma, \; i = 1, 2.$
Then for each $t \in \mathbf{R}$ we define a "canonical vacuum state" by the one-particle Hilbert space structure (see Theorem 3.3)

$$\begin{aligned} k^t : \Gamma &\rightarrow \mathcal{H}^t := L^2_{\mathbf{C}}(\Sigma_t, d^3\sigma) \\ (f, p) &\mapsto \frac{1}{\sqrt{2}} \left(A^{1/4} f - i A^{-1/4} p \right). \end{aligned} \tag{3.29}$$

From [32, 33] it follows:

Theorem 3.13 *For each $t \in \mathbf{R}$, $(k^t, \mathcal{H}^t)$ defines a pure, quasifree state ω_t on the Weyl algebra of the Klein-Gordon field on the globally hyperbolic ultrastatic spacetime $(\mathcal{M}, g)$. ω_t is the unique quasifree ground state with respect to the time translations $t \mapsto t + t_o$ (i.e. in fact independent of t). The one-particle Hamiltonian (Definition 3.4) is $h = A^{1/2}$.*

Let us calculate the ("four-smeared") two-point function of ω_t:
For $h_1, h_2 \in \mathcal{D}(\mathcal{M})$, by equ. (3.14),

$$\Lambda^{(2)}_t(h_1, h_2) = \lambda^{(2)}_t \left(\begin{pmatrix} \rho_o E h_1 \\ \rho_1 E h_1 \end{pmatrix}, \begin{pmatrix} \rho_o E h_2 \\ \rho_1 E h_2 \end{pmatrix} \right), \tag{3.30}$$

where E is the fundamental solution of the Klein-Gordon equation in this spacetime, $\rho_o \Phi := \Phi|_{\Sigma_t}$, $\rho_1 \Phi := \frac{\partial \Phi}{\partial t}|_{\Sigma_t}$, and the "symplectically smeared two-point function" $\lambda_t^{(2)}$ is given on the initial data $F_i = \binom{f_i}{p_i} \in \Gamma$ by equ. (3.13),

$$\begin{aligned}
\lambda_t^{(2)}(F_1, F_2) &= \left\langle k^t F_1, k^t F_2 \right\rangle_{\mathcal{H}^t} \\
&= \frac{1}{2} \left\langle A^{1/4} f_1 - i A^{-1/4} p_1, A^{1/4} f_2 - i A^{-1/4} p_2 \right\rangle_{\mathcal{H}^t} \\
&= \frac{1}{2} \left\langle (A^{1/2} f_1 - i p_1), A^{-1/2} \left(A^{1/2} f_2 - i p_2 \right) \right\rangle_{\mathcal{H}^t}, \qquad (3.31)
\end{aligned}$$

since A is selfadjoint. Combining (3.30) and (3.31) we obtain

$$\Lambda_t^{(2)}(h_1, h_2) = \frac{1}{2} \left\langle \left(A^{1/2} \rho_o - i \rho_1 \right) E h_1, A^{-1/2} \left(A^{1/2} \rho_o - i \rho_1 \right) E h_2 \right\rangle_{\mathcal{H}^t} \qquad (3.32)$$

or in a more transparent integral representation (using $E' = -E$)

$$\Lambda_t^{(2)}(x_1, x_2) = -\frac{1}{2} \int_{\Sigma_t} d^3 y \sqrt{h(\vec{y})}\, \overline{E(x_1; t, \vec{y}) \left(A^{1/2} - i \frac{\overleftarrow{\partial}}{\partial t} \right)} A^{-1/2} \left(A^{1/2} - i \frac{\overrightarrow{\partial}}{\partial t} \right) E(t, \vec{y}; x_2), \qquad (3.33)$$

where A acts on $\vec{y} \in \Sigma_t$. To show that ω_t is a Hadamard state we only have to prove that the two-point distribution (3.33) has the wavefront set (3.24) (Theorem 3.9). To this end, let us be slightly more general than necessary at the moment. This will pay off in the next section where we can apply the same method of proof to the adiabatic vacua.
Let $K_1^t \in \mathcal{D}'(\mathcal{M} \times \Sigma_t)$, $K_2^t \in \mathcal{D}'(\Sigma_t \times \mathcal{M})$ and $\Lambda_t^{(2)} \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be given such that

$$\begin{aligned}
\Lambda_t^{(2)} &= K_1^t \circ K_2^t, \qquad (3.34) \\
K_1^t(x_1, \vec{y}) &:= \overline{\frac{1}{\sqrt{2}} E(x_1; t, \vec{y}) \left(B - i \frac{\overleftarrow{\partial}}{\partial t} \right)} \\
K_2^t(\vec{y}, x_2) &:= -\frac{1}{\sqrt{2}} A \left(B - i \frac{\partial}{\partial t} \right) E(t, \vec{y}; x_2). \qquad (3.35)
\end{aligned}$$

To calculate the wavefront set of the composition (3.34) of two distributions we prove a lemma which amounts to a proof of Theorem 2.23 under somewhat different assumptions:

Lemma 3.14 *If $A(t)$ and $B(t)$ are pseudodifferential operators on Σ_t and $\Lambda_t^{(2)}, K_1^t, K_2^t$ are given as above, then*

$$WF'(\Lambda_t^{(2)}) \subset WF'(K_1^t) \circ WF'(K_2^t). \qquad (3.36)$$

PROOF:
i) Our aim is to apply Theorem 2.23. But we cannot do so directly since our distributions K_1^t and K_2^t are not properly supported. However, since $A \left(B - i \frac{\partial}{\partial t} \right)$ is a pseudodifferential operator we have by the pseudolocal property (Theorem 2.13) and Lemma 2.19a)

$$\begin{aligned}
WF'(K_1^t) &\subset -WF'(E|_{\mathcal{M} \times \Sigma_t}) \subset -\varphi_{2*}^t(C) \\
WF'(K_2^t) &\subset WF'(E|_{\Sigma_t \times \mathcal{M}}) \subset \varphi_{1*}^t(C), \qquad (3.37)
\end{aligned}$$

where $C = WF'(E)$ (see Theorem 2.29a)) is given by equ. (2.41) and the second inclusion follows from Theorem 2.22, φ_1^t, φ_2^t being the imbeddings $\varphi_1^t : \Sigma_t \times \mathcal{M} \to \mathcal{M} \times \mathcal{M}$ and $\varphi_2^t : \mathcal{M} \times \Sigma_t \to \mathcal{M} \times \mathcal{M}$.
Now we observe from (3.37) that K_1^t and K_2^t are properly supported w.r.t. their *singular* support. Therefore we can choose a properly supported $\chi \in \mathcal{C}^\infty(\mathcal{M} \times \Sigma_t)$ with $0 \le \chi \le 1$, $\chi = 1$ in a neighborhood of $singsupp\, E|_{\mathcal{M}\times\Sigma_t}$ and $\psi \in \mathcal{C}^\infty(\Sigma_t \times \mathcal{M})$ with $\psi(\vec{y}, x) := \chi(x, \vec{y})$, $x \in \mathcal{M}$, $\vec{y} \in \Sigma_t$.
Then $K_1^t\chi$ and ψK_2^t are properly supported, whereas $K_1^t(1-\chi)$ and $(1-\psi)K_2^t$ are smooth. We decompose

$$\begin{aligned} \Lambda_t^{(2)} &= (K_1^t\chi) \circ (\psi K_2^t) + K_1^t(1-\chi) \circ (1-\psi)K_2^t \\ &\quad + (K_1^t\chi) \circ (1-\psi)K_2^t + K_1^t(1-\chi) \circ (\psi K_2^t) \\ &=: I_1 + I_2 + I_3 + I_4 \end{aligned}$$

and claim that

$$WF(\Lambda_t^{(2)}) = WF(I_1) \tag{3.38}$$

(which, then, can be calculated from Theorem 2.23). Since I_2 is a composition of smooth distributions it does not contribute to the wavefront set. Let us consider

$$I_4(x_1, x_2) = \int_{\Sigma_t} d^3y \sqrt{h(\vec{y})}\, \left(K_1^t(1-\chi)\right)(x_1, \vec{y})\left(\psi K_2^t\right)(\vec{y}, x_2).$$

Localizing I_4 around x_1 and x_2 and taking the Fourier transform we obtain

$$\hat{I}_4(\xi_1, \xi_2) \int d^3\eta\, [K_1^t(1-\chi)]\hat{\ }(\xi_1, -\eta)(\widehat{\psi K_2^t})(\eta, \xi_2). \tag{3.39}$$

Since ψK_2^t is properly supported the integration over $\vec{y} \in \Sigma_t$ is only over a compact set (which we can assume to be covered by one coordinate patch), hence $\widehat{\psi K_2^t}(\eta, \xi_2)$ is polynomially bounded in $|\eta|$, whereas $[K_1^t(1-\chi)]\hat{\ }(\xi_1, -\eta)$ falls off rapidly in $|\eta|$ because $K_1^t(1-\chi)$ is smooth (which shows the existence of the integral). The integrand of (3.39) can be estimated by

$$C_N(1 + |\xi_1| + |\eta|)^{-N}(1 + |\eta| + |\xi_2|)^k$$

for arbitrary N and some fixed k. If $\epsilon > 0$ it follows that $\hat{I}_4(\xi_1, \xi_2)$ is rapidly decreasing when either $|\xi_1| > \epsilon|\xi_2|$ or $|\eta| > \epsilon|\xi_2|$. Thus, by Theorem 2.18, the wavefront set of I_4 is certainly contained in the set where this is not the case, namely

$$\begin{aligned} WF(I_4) &\subset \{(x_1, 0; x_2, \xi_2) \in T^*(\mathcal{M} \times \mathcal{M});\ (y, 0; x_2, \xi_2) \in WF(E|_{\Sigma_t\times\mathcal{M}}) \text{ for some } y \in \Sigma_t\} \\ &= \mathcal{M} \times WF_{\mathcal{M}}(E|_{\Sigma_t\times\mathcal{M}}) \end{aligned}$$

(see equ. (2.34)) which is however empty, as we shall find out in a moment. Hence I_4 and (analogously) I_3 do not contribute to $WF(\Lambda_t^{(2)})$, i.e. it holds (3.38) as claimed.
ii) Since I_1 is the composition of two properly supported distributions having the same singular points as K_1^t and K_2^t we obtain from (3.38) and Theorem 2.23

$$\begin{aligned} WF'(\Lambda_t^{(2)}) &= WF'(I_1) \\ &\subset WF'(K_1^t) \circ WF'(K_2^t) \cup (WF_{\mathcal{M}}(K_1^t) \times \mathcal{M}) \cup (\mathcal{M} \times WF'_{\mathcal{M}}(K_2^t)). \end{aligned}$$

Now, by the defining equ. (2.34) and (3.37),

$$\begin{aligned}
WF_{\mathcal{M}}(K_1^t) &= \{(x_1,\xi_1)\in T^*\mathcal{M};\ (x_1,\xi_1;y,0)\in WF(K_1^t) \text{ for some } y\in\Sigma_t\} \\
&\subset \{(x_1,\xi_1)\in T^*\mathcal{M};\ (x_1,\xi_1;y,0)\in -\varphi^t_{2*}(C) \text{ for some } y\in\Sigma_t\} \\
&= \emptyset
\end{aligned}$$

by inspection of C (equ. (2.41)) and similarly,

$$WF'_{\mathcal{M}}(K_2^t)=\emptyset,$$

hence $WF'(\Lambda_t^{(2)})\subset WF'(K_1^t)\circ WF'(K_2^t)$ which was to be proved. □

Now, with formula (3.36) at hand, we can calculate the wavefront set of $\Lambda_t^{(2)}$. The next theorem contains one of the main results of this work. It gives a sufficient criterion for a quasifree state to be an Hadamard state. The idea is to use – instead of positive frequency solutions of the Klein-Gordon equation – a separation of the Klein-Gordon operator into first order factors that project out the positive frequency parts of the fundamental solution:

Theorem 3.15 *Let $A(t)$ be an elliptic pseudodifferential operator on Σ_t. Let $B(t)$ be a pseudodifferential operator on Σ_t such that there exists a pseudodifferential operator Q on $\mathcal{M}$ which has the property $Q(B-i\partial_t)=\Box_g+\mu^2$ and possesses a principal symbol q with*

$$q^{-1}(0)\setminus\{0\}\subset\{(x,\xi)\in T^*\mathcal{M};\ \xi^0>0\}. \tag{3.40}$$

Let the two-point distribution $\Lambda_t^{(2)}\in\mathcal{D}'(\mathcal{M}\times\mathcal{M})$ of a quasifree state be given by

$$\Lambda_t^{(2)}(h_1,h_2)=\frac{1}{2}\langle(B-i\partial_t)Eh_1,A(B-i\partial_t)Eh_2\rangle_{L^2_{\mathbb{C}}(\Sigma_t,d^3\sigma)} \tag{3.41}$$

or in integral representation

$$\Lambda_t^{(2)}(x_1,x_2)=-\frac{1}{2}\int_{\Sigma_t}d^3y\sqrt{h(t,\vec{y})}\,\overline{E(x_1;t,\vec{y})\left(B-i\overleftarrow{\partial_t}\right)}A\left(B-i\overrightarrow{\partial_t}\right)E(t,\vec{y};x_2) \tag{3.42}$$

where A,B act on $\vec{y}\in\Sigma_t$.
Then the wavefront set of $\Lambda_t^{(2)}$ is given by that of an Hadamard distribution, namely

$$WF(\Lambda_t^{(2)})=\{(x_1,\xi_1;x_2,-\xi_2)\in T^*(\mathcal{M}\times\mathcal{M})\setminus\{0\};\ (x_1,\xi_1)\sim(x_2,\xi_2),\xi_1^0\geq 0\}$$

(see Theorem 3.9).

PROOF:
i) Since $\Lambda_t^{(2)}$ is the two-point distribution of a quasifree state its imaginary part must be proportional to the fundamental solution E (by equ. (3.15)), and hence

$$singsupp\, E\subset singsupp\,\Lambda_t^{(2)},$$

i.e. $WF(\Lambda_t^{(2)})$ is not empty.
ii) $\Lambda_t^{(2)}$ is Hermitean in the sense that $\Lambda_t^{(2)}(x_1,x_2)=\overline{\Lambda_t^{(2)}(x_2,x_1)}$. Therefore (by Lemma 2.19b)) the wavefront set must be Hermitean in the sense

$$(x_1,\xi_1;x_2,\xi_2)\in WF(\Lambda_t^{(2)})\Leftrightarrow(x_2,-\xi_2;x_1,-\xi_1)\in WF(\Lambda_t^{(2)}),$$

i.e. $WF'(\Lambda_t^{(2)})$ must be symmetric.
iii) $\Lambda_t^{(2)}$ is a solution of the Klein-Gordon equation in both arguments, i.e. $\forall h_1, h_2 \in \mathcal{D}(\mathcal{M})$

$$\Lambda_t^{(2)}((\Box_g + \mu^2)h_1, h_2) = \Lambda_t^{(2)}(h_1, (\Box_g + \mu^2)h_2) = 0,$$

therefore we can apply Theorem 2.17 to conclude that

$$WF(\Lambda_t^{(2)}) \subset N \times N,$$

where $N := \{(x,\xi) \in T^*\mathcal{M}\backslash\{0\};\ g^{\mu\nu}\xi_\mu\xi_\nu = 0\}$ was already defined in equ. (2.39), and $WF(\Lambda_t^{(2)})$ must be invariant under the Hamiltonian vectorfield (2.40) (propagation of singularities), i.e.

$$\left.\begin{array}{c}(x_1,\xi_1;x_2,\xi_2) \in WF(\Lambda_t^{(2)}) \\ (x_2,\xi_2) \sim (x_2',\xi_2')\end{array}\right\} \Rightarrow (x_1,\xi_1;x_2',\xi_2') \in WF(\Lambda_t^{(2)})$$
$$\left.\begin{array}{c}(x_1,\xi_1;x_2,\xi_2) \in WF(\Lambda_t^{(2)}) \\ (x_1,\xi_1) \sim (x_1',\xi_1')\end{array}\right\} \Rightarrow (x_1',\xi_1';x_2,\xi_2) \in WF(\Lambda_t^{(2)}).$$

iv) To see that singularities can only occur on the lightcone let us look at the initial data of $\Lambda_t^{(2)}$ on $\Sigma \times \Sigma$. Using equations (3.7) we calculate from (3.42)

$$\begin{aligned}
\Lambda_t^{(2)}|_{\Sigma_t\times\Sigma_t}(f_1,f_2) &= \frac{1}{2}\langle f_1, Af_2\rangle \\
\left(\frac{\partial}{\partial x_1^0} \otimes \mathbf{1}\right)\Lambda_t^{(2)}|_{\Sigma_t\times\Sigma_t}(f_1,f_2) &= \frac{i}{2}\langle f_1, BAf_2\rangle \\
\left(\mathbf{1} \otimes \frac{\partial}{\partial x_2^0}\right)\Lambda_t^{(2)}|_{\Sigma_t\times\Sigma_t}(f_1,f_2) &= \frac{i}{2}\langle f_1, ABf_2\rangle \\
\left(\frac{\partial}{\partial x_1^0} \otimes \frac{\partial}{\partial x_2^0}\right)\Lambda_t^{(2)}|_{\Sigma_t\times\Sigma_t}(f_1,f_2) &= \frac{1}{2}\langle f_1, BABf_2\rangle
\end{aligned} \tag{3.43}$$

for $f_1, f_2 \in \mathcal{D}(\Sigma_t)$, i.e. the initial data are (proportional to) the kernel distributions of pseudodifferential operators and hence, by Lemma 2.6, singular only on the diagonal of $\Sigma_t \times \Sigma_t$. Therefore, by the propagation of singularities iii), singularities can only occur if x_1 and x_2 are lightlike connected.
Summarizing i)–iv) we can conclude that $WF(\Lambda_t^{(2)})$ must be a non-empty subset of $\{(x_1,\xi_1;x_2,\xi_2) \in N \times N;\ x_1$ and x_2 are lightlike connected$\}$ which is invariant under the Hamiltonian vectorfield and Hermitean.
v) Now we are going to apply Lemma 3.14.
Let K_1^t and K_2^t be defined as in (3.35). First note, that by Theorem 2.16, Theorem 2.22 and Lemma 2.19

$$\begin{aligned}
WF'(K_1^t) &= WF'(\overline{(B-i\partial_t)E|_{\mathcal{M}\times\Sigma_t}}) \subset -\varphi_{2*}^t WF'((\mathbf{1}\otimes P)E) \\
WF'(K_2^t) &= WF'((B-i\partial_t)E|_{\Sigma_t\times\mathcal{M}}) \subset \varphi_{1*}^t WF'((P\otimes\mathbf{1})E)
\end{aligned} \tag{3.44}$$

because A is an elliptic pseudodifferential operator (we have set $P := B - i\partial_t$). Then decompose E into distinguished parametrices (see Theorem 2.28)

$$\begin{aligned}
E &= \Delta_R - \Delta_A \\
&= (\Delta_F - \Delta_A) + (\Delta_R - \Delta_F) \\
&=: E^+ + E^-,
\end{aligned}$$

where, by Theorem 2.29 and the pseudolocal property (Theorem 2.13),

$$\begin{aligned} WF'((P \otimes \mathbf{1})E^-) &\subset WF'(E^-) = C \cap (N'_- \times N'_-) \\ WF'((\mathbf{1} \otimes P)E^+) &\subset WF'(E^+) = C \cap (N'_+ \times N'_+). \end{aligned} \tag{3.45}$$

Now the essential observation is that

$$\begin{aligned} (QP \otimes \mathbf{1})E^- &= ((\Box_g + \mu^2) \otimes \mathbf{1})E^- \\ &= ((\Box_g + \mu^2) \otimes \mathbf{1})(\Delta_R - \Delta_F) = 0 \, (mod\, \mathcal{C}^\infty) \\ (\mathbf{1} \otimes QP)E^+ &= (\mathbf{1} \otimes (\Box_g + \mu^2))(\Delta_F - \Delta_A) = 0 \, (mod\, \mathcal{C}^\infty), \end{aligned} \tag{3.46}$$

since Δ_F, Δ_R and Δ_A are parametrices of $(\Box_g + \mu^2)$. Therefore, by Theorem 2.17 and (3.45), and using the assumption $q^{-1}(0) \setminus \{0\} \subset \{(x,\xi) \in T^*\mathcal{M};\ \xi^0 > 0\}$,

$$\begin{aligned} WF'((P \otimes \mathbf{1})E^-) &\subset C \cap (N'_- \times N'_-) \cap (q^{-1}(0) \times T^*\mathcal{M}) = \emptyset \\ WF'((\mathbf{1} \otimes P)E^+) &\subset C \cap (N'_+ \times N'_+) \cap (T^*\mathcal{M} \times -q^{-1}(0)) = \emptyset, \end{aligned} \tag{3.47}$$

whereas

$$\begin{aligned} WF'((P \otimes \mathbf{1})E^+) &\subset C \cap (N'_+ \times N'_+) \\ WF'((\mathbf{1} \otimes P)E^-) &\subset C \cap (N'_- \times N'_-) \end{aligned} \tag{3.48}$$

by the pseudolocal property. Now we apply Lemma 3.14 to obtain from equations (3.44), (3.47) and (3.48)

$$\begin{aligned} WF'(\Lambda_t^{(2)}) &\subset WF'(K_1^t) \circ WF'(K_2^t) \\ &\subset -\varphi_{2*}^t WF'((\mathbf{1} \otimes P)(E^+ + E^-)) \circ \varphi_{1*}^t WF'((P \otimes \mathbf{1})(E^+ + E^-)) \\ &\subset \varphi_{2*}^t (C \cap (N'_+ \times N'_+)) \circ \varphi_{1*}^t (C \cap (N'_+ \times N'_+)) \\ &\subset C \cap (N'_+ \times N'_+). \end{aligned}$$

Together with i)–iv) we obtain $WF'(\Lambda_t^{(2)}) = C \cap (N'_+ \times N'_+)$, which is the wavefront set of an Hadamard distribution as was to be proven. □

As an immediate consequence of Theorem 3.15 we can now prove that the ultrastatic vacua defined by (3.29) are Hadamard states:

Corollary 3.16 *Let $(\mathcal{M}, g)$ be an ultrastatic globally hyperbolic spacetime which is foliated by compact spacelike Cauchy surfaces Σ_t.*
Let ω be the quasifree ground state of the Klein-Gordon quantum field on $(\mathcal{M}, g)$ as defined by (3.29) and Theorem 3.13.
Then ω is an Hadamard state.

PROOF:
Looking at the two-point distribution (3.33) of ω it is clear that it only remains to be shown that $A^{\pm 1/2}$ has the properties which are demanded in Theorem 3.15.
But since $A = \overline{-{}^{(3)}\Delta_h + \mu^2}$ is an elliptic, selfadjoint operator and Σ_t compact we can apply

Theorem 2.25 to conclude that $A^{\pm 1/2}$ is an elliptic pseudodifferential operator with principal symbol $(h^{ij}\xi_i\xi_j)^{\pm 1/2}$ of order 1. Furthermore $Q := A^{1/2}+i\partial_t$ is a pseudodifferential operator with principal symbol $q = (h^{ij}\xi_i\xi_j)^{1/2}-\xi_0$, i.e. it satisfies (3.40), and $Q(A^{1/2}-i\partial_t) = A+\partial_t^2 = \Box_g+\mu^2$, since, on an ultrastatic spacetime, A is independent of t. $\Box$

Remarks:

1. The restriction in the corollary to compact Cauchy surfaces has the technical reason that only for those Theorem 2.25 is formulated in the mathematical literature. In fact, Corollary 3.16 also holds in the non-compact case as was proven in [22].

2. The statement of the corollary also holds for static spacetimes (3.26) on which the norm of the timelike Killing field t^μ is bounded from below by a positive constant ϵ:

$$\alpha(\vec{x})^2 = g_{\mu\nu}(x)t^\mu t^\nu \geq \epsilon > 0 \; \forall \; x \in \mathcal{M}. \tag{3.49}$$

   In this case, the two-point function of the groundstate reads [32]

$$\Lambda^{(2)}(h_1, h_2) = \frac{1}{2}\langle (B - \frac{i}{\alpha}\partial_t)Eh_1, B^{-1}(B - \frac{i}{\alpha}\partial_t)Eh_2\rangle_{\mathcal{H}^t}$$

   with

$$\begin{aligned} B &:= \alpha^{-1/2}(\alpha^{1/2}\bar{A}\alpha^{1/2})^{1/2}\alpha^{-1/2} \\ A &:= -(\partial^i\alpha)\partial_i + \alpha(-{}^{(3)}\Delta_h + \mu^2) \end{aligned}$$

   and it holds

$$\frac{1}{\alpha}(i\partial_t + B\alpha)(B - \frac{i}{\alpha}\partial_t) = \frac{1}{\alpha^2}\partial_t^2 + \frac{1}{\alpha}A = \Box_g + \mu^2.$$

   Since pseudodifferential operators commute in highest order the principal symbol of B is again $(h^{ij}\xi_i\xi_j)^{1/2}$ and the proof from above carries over immediately.

3. Condition (3.49) however cannot be relaxed further, since e.g. the ground state w.r.t. the static Killing field in the Schwarzschild metric ("Boulware vacuum") is known to be not a Hadamard state [38]. There, (3.49) is violated on the horizon, and the mathematical analysis from above breaks down since the corresponding operator is no longer elliptic.

4. Similar statements for stationary spacetimes (i.e. spacetimes with a timelike Killing field which is not necessarily hypersurface-orthogonal) are not known since the two-point function of the ground state (see [32]) cannot be represented by such an explicit formula like (3.33).

Let us consider next the KMS-states arising when one "heats up" the ground state (3.29) to a temperature $T = 1/\beta$. Kay [35] shows how one can construct quasifree KMS-states from a given quasifree groundstate:
Let $(k, \mathcal{H}, e^{-iht})$ be a one-particle Hilbertspace structure of a quasifree groundstate (Definition 3.4) over a phase space $(\Gamma, \sigma, \mathcal{T}(t))$ such that $k\Gamma \subset \mathcal{D}(h^{-1/2})$ (what Kay calls "regularity

condition"). Then a one-particle structure for a quasifree KMS-state at temperature $T = 1/\beta$ is given by $(k^\beta, \tilde{\mathcal{H}}, e^{-i\tilde{h}t})$ as follows:

$$
\begin{aligned}
k^\beta : \Gamma &\rightarrow \tilde{\mathcal{H}} := \mathcal{H} \oplus \mathcal{H} \\
F &\mapsto C(\sinh Z^\beta)kF \oplus (\cosh Z^\beta)kF, \\
e^{-i\tilde{h}t} &= \begin{pmatrix} e^{ith} & 0 \\ 0 & e^{-ith} \end{pmatrix},
\end{aligned}
\tag{3.50}
$$

where Z^β is implicitly defined by $\tanh Z^\beta = e^{-\beta h}$, i.e.

$$
\sinh Z^\beta = \frac{e^{-\beta h/2}}{(1-e^{-\beta h})^{1/2}}, \ \cosh Z^\beta = \frac{1}{(1-e^{-\beta h})^{1/2}},
$$

and $C : \mathcal{H} \rightarrow \mathcal{H}$ is a complex conjugation such that $Ce^{-ith} = e^{ith}C$. Since $\mathcal{D}(h^{-1/2}) \subset \mathcal{D}(\sinh Z^\beta), \mathcal{D}(\cosh Z^\beta)$ (see [35]) the regularity condition guarantees that (3.50) is well defined.

In our case of the ultrastatic groundstate (3.29) the regularity condition is satisfied since $A^{1/4}\mathcal{C}_o^\infty(\Sigma_t) \subset A^{1/4}\mathcal{D}(A^{1/2}) \subset \mathcal{D}(A^{-1/4}) = \mathcal{D}(h^{-1/2})$ and $A^{-1/4}\mathcal{C}_o^\infty(\Sigma_t) \subset A^{-1/4}\mathcal{D}(A^{-1/2}) \subset \mathcal{D}(A^{-1/4}) = \mathcal{D}(h^{-1/2})$. Representing C by the ordinary complex conjugation on $\mathcal{H} = L^2_{\mathbf{C}}(\Sigma_t, d^3\sigma)$ we can compute the two-point function (3.13), (3.14) of an ultrastatic KMS-state as

$$
\begin{aligned}
\lambda_\beta^{(2)}(F_1, F_2) &= \langle k^\beta F_1, k^\beta F_2 \rangle_{\tilde{\mathcal{H}}} \\
&= \frac{1}{2}\Big\{\langle C(\sinh Z^\beta)(A^{1/4}f_1 - iA^{-1/4}p_1), C(\sinh Z^\beta)(A^{1/4}f_2 - iA^{-1/4}p_2)\rangle_{\mathcal{H}} \\
&\quad + \langle(\cosh Z^\beta)(A^{1/4} - iA^{-1/4}p_1), (\cosh Z^\beta)(A^{1/4}f_2 - iA^{-1/4}p_2)\rangle_{\mathcal{H}}\Big\} \\
&= \frac{1}{2}\Big\{\langle(A^{1/2}f_1 + ip_1), (\sinh^2 Z^\beta)A^{-1/2}(A^{1/2}f_2 + ip_2)\rangle_{\mathcal{H}} \\
&\quad + \langle(A^{1/2}f_1 - ip_1), (\cosh^2 Z^\beta)A^{-1/2}(A^{1/2}f_2 - ip_2)\rangle_{\mathcal{H}}\Big\}
\end{aligned}
\tag{3.51}
$$

for $F_i = (f_i, p_i) \in \Gamma = \mathcal{C}_o^\infty(\Sigma_t) \oplus \mathcal{C}_o^\infty(\Sigma_t)$, using the selfadjointness of A, and

$$
\begin{aligned}
\Lambda_\beta^{(2)}(h_1, h_2) &= \frac{1}{2}\Big\{\langle(A^{1/2} + i\partial_t)Eh_1, (\sinh^2 Z^\beta)A^{-1/2}(A^{1/2} + i\partial_t)Eh_2\rangle_{\mathcal{H}} \\
&\quad + \langle(A^{1/2} - i\partial_t)Eh_1, (\cosh^2 Z^\beta)A^{-1/2}(A^{1/2} - i\partial_t)Eh_2\rangle_{\mathcal{H}}\Big\}
\end{aligned}
\tag{3.52}
$$

for $h_i \in \mathcal{D}(\mathcal{M}), i = 1, 2$, and we claim:

Corollary 3.17 *Let $(\mathcal{M}, g)$ be an ultrastatic globally hyperbolic spacetime with compact spacelike Cauchy surfaces Σ_t. Let ω_β be the quasifree KMS-state ($\beta > 0$) of the Klein-Gordon quantum field on $(\mathcal{M}, g)$ as defined by (3.50).*
Then ω_β is an Hadamard state.

PROOF:
Let us look at the two-point function (3.52). The second term in (3.52) is again of the form (3.41), but with the operator A in the middle replaced by

$$
(\cosh^2 Z^\beta)A^{-1/2} = \frac{A^{-1/2}}{1 - e^{-\beta A^{1/2}}},
$$

which is, by Theorem 2.25, an elliptic pseudodifferential operator. Hence the second term contributes to $\Lambda^{(2)}_\beta$ the wavefront set of an Hadamard distribution, whereas the first term is in fact smooth:
Using (3.7) we can compute the distributional initial data of the first term in (3.52) obtaining distributions which have as kernels the pseudodifferential operators $(\sinh^2 Z^\beta)A^{1/2}$, $\sinh^2 Z^\beta$ and $(\sinh^2 Z^\beta)A^{-1/2}$. But noting that

$$\sinh^2 Z^\beta = \frac{e^{-\beta A^{1/2}}}{1 - e^{-\beta A^{1/2}}}$$

and using again Theorem 2.25 we see that the principal symbols of these operators fall off faster than any inverse power in ξ. Therefore, by Lemma 2.6b), these distributions have smooth kernels, and, consequently, so has the first term of (3.52). □

Remark:
This result seems to be new. As for the groundstate, it also immediately extends to the case of a static metric satisfying (3.49).

3.4 Adiabatic vacua on Robertson-Walker spaces

Adiabatic vacua were introduced by Parker [45, 46] in order to investigate the particle production in the expanding universe. A mathematically precise definition was given by Lüders and Roberts [41]. In the following we will define adiabatic vacua following [41] and review this paper as far as it is necessary for our purposes. Then we will state and prove one of the main results of this work, namely that all adiabatic vacuum states are Hadamard states.
The homogeneous and isotropic spacetimes are the Lorentz manifolds of the form $\mathcal{M}^\kappa = \mathbf{R} \times \Sigma^\kappa$, $\kappa = -1, 0, +1$, endowed with the **Robertson-Walker metrics**

$$ds^2 = dt^2 - a(t)^2 \left[\frac{dr^2}{1 - \kappa r^2} + r^2 (d\theta^2 + \sin^2\theta d\varphi^2) \right] \tag{3.53}$$

($\varphi \in [0, 2\pi], \theta \in [0, \pi], r \in [0, \infty)$ for $\kappa = 0, -1$, $r \in [0, 1)$ for $\kappa = +1$), where a is a strictly positive smooth function and Σ^κ a homogeneous Riemannian manifold with constant negative ($\kappa = -1$), positive ($\kappa = +1$) or zero ($\kappa = 0$) curvature. Choosing the simplest topologies for Σ^κ we can regard Σ^κ as being embedded in $\mathbf{R}^4$:

$$\begin{aligned} \Sigma^+ &= \{x \in \mathbf{R}^4;\ (x^0)^2 + \sum_{i=1}^{3} (x^i)^2 = 1\}, \\ \Sigma^0 &= \{x \in \mathbf{R}^4;\ x^0 = 0\}, \\ \Sigma^- &= \{x \in \mathbf{R}^4;\ (x^0)^2 - \sum_{i=1}^{3} (x^i)^2 = 1, x^0 > 0\}. \end{aligned} \tag{3.54}$$

Since Σ^+ is compact $\mathcal{M}^+$ is called a "closed" universe, whereas $\mathcal{M}^0$ and $\mathcal{M}^-$ are models for "open" universes having noncompact spatial sections. (For an interpretation of these as cosmological models see e.g. [59].) The Riemannian metric

$$s^\kappa_{ij} = \begin{pmatrix} \frac{1}{1-\kappa r^2} & & \\ & r^2 & \\ & & r^2 \sin^2\theta \end{pmatrix} \tag{3.55}$$

is induced on Σ^κ by the Euclidean metric on $\mathbf{R}^4$ for $\kappa = +1, 0$ and the Minkowski metric for $\kappa = -1$. These spaces are homogeneous for the rotation group SO(4) ($\kappa = +1$), the Euclidean group E(3) ($\kappa = 0$), resp. the Lorentz group $\mathcal{L}_+^\uparrow(4)$ ($\kappa = -1$).
The $\mathcal{M}^\kappa$ are globally hyperbolic and the hypersurfaces $\Sigma_t^\kappa := \{t\} \times \Sigma^\kappa$ are Cauchy surfaces of $\mathcal{M}^\kappa$ with 3-metric $h_{ij}^\kappa = a^2(t) s_{ij}^\kappa$. Their future-directed normal field is given by $n^\alpha = (1, 0, 0, 0)$. It is geodesic ($n^\alpha \nabla_\alpha n^\beta = 0$). The exterior curvature K of Σ_t^κ is

$$K = \nabla_\alpha n^\alpha = 3 \frac{\dot{a}(t)}{a(t)}. \tag{3.56}$$

In what follows we will omit the index κ unless it is necessary to specify one of its values.
We want to consider linear scalar fields on these spaces and therefore have to study the Klein-Gordon equation in the background (3.53)

$$(\Box_g + \mu^2)\Phi = \frac{\partial^2 \Phi}{\partial t^2} + 3 \frac{\dot{a}}{a} \frac{\partial \Phi}{\partial t} + (-{}^{(3)}\Delta_h + \mu^2)\Phi = 0, \tag{3.57}$$

where ${}^{(3)}\Delta_h$ is the Laplace-Beltrami operator on Σ_t,

$$\begin{aligned} {}^{(3)}\Delta_h &= \frac{1}{a^2} \left\{ (1 - \kappa r^2) \frac{\partial^2}{\partial r^2} + \frac{2 - 3\kappa r^2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta(\theta, \varphi) \right\} \\ \Delta(\theta, \varphi) &:= \frac{1}{\sin\theta} \left[\frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \cdot \right) + \frac{1}{\sin\theta} \frac{\partial^2}{\partial \varphi^2} \cdot \right]. \end{aligned} \tag{3.58}$$

The partial differential equation (3.57) can be separated by

$$\Phi(t, r, \theta, \varphi) = \int d\mu(\vec{k})\, T_{\vec{k}}(t) \phi_{\vec{k}}(r, \theta, \varphi)$$

into an ordinary differential equation for the time dependent part $T_{\vec{k}}(t)$

$$\ddot{T}_{\vec{k}} + 3 \frac{\dot{a}}{a} \dot{T}_{\vec{k}} + \omega_k^2 T_{\vec{k}} = 0 \tag{3.59}$$

where

$$\omega_k^2(t) := \frac{E(k)}{a^2(t)} + \mu^2 \tag{3.60}$$

and eigenfunctions $\phi_{\vec{k}}(r, \theta, \varphi)$ of the Laplace-Beltrami operator on a hypersurface Σ_t:

$${}^{(3)}\Delta_h \phi_{\vec{k}} = -\frac{E(k)}{a^2} \phi_{\vec{k}}. \tag{3.61}$$

(Note that ${}^{(3)}\Delta_h$, equ. (3.58), is of the form $\frac{1}{a^2}\tilde{\Delta}$, where $\tilde{\Delta}$ is the Laplace-Beltrami operator of s_{ij}, equ. (3.55), so the $\phi_{\vec{k}}$ live in fact on Σ and are independent of t.) The notation we have used is the following:

$$\begin{aligned} \int d\mu(\vec{k}) &:= \sum_{k=0}^{\infty} \sum_{l=0}^{k} \sum_{m=-l}^{l}, \ \vec{k} := (k, l, m), \ E(k) := k(k+2) \text{ for } \kappa = +1 \\ \int d\mu(\vec{k}) &:= \int_{\mathbf{R}^3} d^3k, \ \vec{k} := (k_1, k_2, k_3) \in \mathbf{R}^3, \ k := |\vec{k}|, \ E(k) := k^2 \text{ for } \kappa = 0 \\ \int d\mu(\vec{k}) &:= \int_{\mathbf{R}^3} d^3k, \ \vec{k} \in \mathbf{R}^3, \ k := |\vec{k}|, \ E(k) := k^2 + 1 \text{ for } \kappa = -1. \end{aligned} \tag{3.62}$$

The (generalized) eigenfunctions $\phi_{\vec{k}}(r,\theta,\varphi)$ are $\frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\vec{x}}$ for $\kappa = 0$, $A_{kl}\Pi^{+}_{kl}(r)Y_{lm}(\theta,\varphi)$ for $\kappa = +1$ (where the Y_{lm} are the spherical harmonics on the two-sphere, $\Pi^{+}_{kl}(r)$ are related to the Gegenbauer polynomials and A_{kl} are normalization constants) and $\frac{1}{(2\pi)^{3/2}}(x\xi)^{-1+ik}$ for $\kappa = -1$ (where $\xi := (1,\vec{\xi})$, $\vec{\xi} := \frac{\vec{k}}{|\vec{k}|}$, $x\xi = x^0 - \vec{x}\vec{\xi} = \sqrt{1+r^2} - \vec{x}\vec{\xi}$). For details see [41]. In each case the system of eigenfunctions is orthonormal and complete, i.e. we can define a generalized Fourier transform by

$$\begin{aligned} \tilde{}: L^2(\Sigma) &\rightarrow L^2(\tilde{\Sigma}) \\ h &\mapsto \tilde{h}(\vec{k}) := (\phi_{\vec{k}}, h) \equiv \int_\Sigma d^3\sigma\, \overline{\phi_{\vec{k}}(\vec{y})} h(\vec{y}), \end{aligned} \tag{3.63}$$

with $d^3\sigma := \sqrt{|s|}d^3y = \frac{1}{\sqrt{1-\kappa r^2}} r^2 dr \sin\theta d\theta d\varphi$ and $\tilde{\Sigma}$ the momentum space associated to Σ (i.e. the range of values of $\vec{k}$ equipped with the measure $d\mu(\vec{k})$). The inverse is given by

$$h(\vec{y}) = \int d\mu(\vec{k})\phi_{\vec{k}}(\vec{y})\tilde{h}(\vec{k}). \tag{3.64}$$

(Note that (3.63) is defined on Σ and not on the Cauchy surface Σ_t.)
We consider the phase space (Γ,σ) of initial data $\Gamma := \mathcal{C}^\infty_o(\Sigma) \oplus a^3\mathcal{C}^\infty_o(\Sigma)$ on Σ with the symplectic form

$$\sigma(F_1,F_2) = -a^3 \int_\Sigma d^3\sigma\, [f_1p_2 - p_1f_2]$$

for $F_i := \binom{f_i}{a^3p_i} \in \Gamma, i = 1,2$, and the Weyl algebra of the linear scalar field associated with (Γ,σ)[1].

Theorem 3.18 (Lüders and Roberts [41]) *The homogeneous and isotropic Fock states for the free Klein-Gordon field in a Robertson-Walker spacetime are given by the following two equivalent constructions:*

a) a two-point function

$$\lambda^{(2)}(F_1,F_2) = \int d\mu(\vec{k})\langle\overline{\tilde{F}_1(\vec{k})}, S(k)\tilde{F}_2(\vec{k})\rangle \tag{3.65}$$

$$S(k) := \begin{pmatrix} |p(k)|^2 & -q(k)\overline{p(k)} \\ -\overline{q(k)}p(k) & |q(k)|^2 \end{pmatrix}, \tag{3.66}$$

where $p(k)$ and $q(k)$ are (essentially polynomially bounded measurable) complex valued functions satisfying

$$\overline{q(k)}p(k) - q(k)\overline{p(k)} = -i. \tag{3.67}$$

b) a representation of the field operators

$$\hat{\Phi}(t,\vec{x}) = \int d\mu(\vec{k})\,[a(\vec{k})\phi_{\vec{k}}(\vec{x})\overline{T_k(t)} + a^*(\vec{k})\overline{\phi_{\vec{k}}(\vec{x})}T_k(t)] \tag{3.68}$$

[1] We insert the factor $a^3(t)$ in the second component of the initial data to comply with the conventions of [41]. We differ from [41] in so far as they use a phase space with elements $F := (a^3p, -f)$.

on a bosonic Fock space with one-particle space $L^2(\tilde{\Sigma})$ and annihilation and creation operators a and a^*,

$$[a(\tilde{f}_1), a^*(\tilde{f}_2)] = \int d\mu(\vec{k})\, \overline{\tilde{f}_1(\vec{k})}\tilde{f}_2(\vec{k}),\ \textit{for}\ \tilde{f}_1, \tilde{f}_2 \in L^2(\tilde{\Sigma}),$$

where the complex valued functions $T_k(t)$ have to obey the differential equation (3.59) and the constraint

$$\overline{T_k}\dot{T}_k - T_k\dot{\overline{T_k}} = -\frac{i}{a^3}. \tag{3.69}$$

Remarks:

1. That the such defined Fock states are homogeneous and isotropic can be read off from the facts that they are constructed w.r.t. the homogeneous surfaces Σ and that $S(k)$ resp. $T_k(t)$ do not depend on the full vectors $\vec{k}$, but only on the norm $k = |\vec{k}|$ (as defined in (3.62)).

2. The conditions (3.67) resp. (3.69) guarantee that the antisymmetric part of $\lambda^{(2)}$ is $i/2$ times the symplectic form σ (which is a necessary condition for two-point functions of quasifree states according to equ. (3.13)).

3. The step from b) to a) is the usual way of constructing Fock states via mode decomposition of the field operators (see e.g. [5]). Since $T_k(t)$ obeys (3.59) the field (3.68) is a (distributional) solution of the Klein-Gordon equation (3.57). Therefore, starting from (3.68) we may define a representation of the field ϑ and its canonical conjugate momentum $\pi := \sqrt{|g|}\frac{\partial\Phi}{\partial t}$ on a Cauchy surface Σ_t and obtain for a testfunction $f \in \mathcal{D}(\mathcal{M})$ (see Theorem 3.1b))

   $$\hat{\Phi}(f) = \vartheta(a^3\rho_1 Ef) - \pi(\rho_o Ef).$$

   Putting $F_i := \binom{\rho_o Ef_i}{a^3\rho_1 Ef_i} \in \Gamma, i = 1, 2$, and defining the Fock state by $a(\vec{k})|0\rangle = 0$ we can calculate the two-point function as

   $$\Lambda^{(2)}(f_1, f_2) = \langle 0|\Phi(f_1)\Phi(f_2)|0\rangle = \int d\mu(\vec{k}) \left\langle \overline{\tilde{F}_1(\vec{k})}, \begin{pmatrix} a^6\overline{\dot{T}_k}\dot{T}_k & -a^3\overline{\dot{T}_k}T_k \\ -a^3\overline{T_k}\dot{T}_k & \overline{T_k}T_k \end{pmatrix} \tilde{F}_2(\vec{k}) \right\rangle.$$

   Comparing with (3.66) we see that $p(k)$ and $q(k)$ are (proportional to) the initial data of $T_k(t)$ on the Cauchy surface Σ_t.

4. The conclusion from a) to b) is proven in [41] imposing a certain continuity condition on the two-point function $\lambda^{(2)}$. The Fock representation (3.68) is constructed from (3.66) in such a way that $T_k(t)$ is a solution of (3.59) with initial data given by $p(k)$ and $q(k)$. (3.69) follows from (3.67) initially at a time t_o, say. But then it holds for all times, because putting $G(t) := \overline{T_k}\dot{T}_k - T_k\dot{\overline{T_k}} + \frac{i}{a^3}$ we obtain from (3.59) $\dot{G}_k(t) + 3\frac{\dot{a}}{a}G_k(t) = 0$ which yields, together with $G_k(t_o) = 0$, that $G_k(t) \equiv 0$ for all t.

As we have seen, the only freedom in the choice of certain homogeneous and isotropic Fock states is the choice of initial data for the function $T_k(t)$. Parker's [45, 46] physical motivation for the definition of the adiabatic vacua was to choose $T_k(t)$ such as to minimize the particle creation in the expanding universe. He achieved this by the use of a WKB-expansion around the ultrastatic groundstate (which only exists if $a(t) = const.$). The formal definition is according to [41]:

Definition 3.19 *An* **adiabatic vacuum state of order** n *is a homogeneous, isotropic Fock state whose two-point function (3.65) is given by functions* $q(k) := T_k(t), p(k) := a^3\dot{T}_k(t)$ *where* $T_k(t)$ *is a solution of the differential equation (3.59) with initial conditions at time* t

$$\begin{aligned} T_k(t) &= W_k^{(n)}(t) \\ \dot{T}_k(t) &= \dot{W}_k^{(n)}(t). \end{aligned} \tag{3.70}$$

Here,

$$W_k^{(n)}(t) := \frac{1}{a^{3/2}(t)\sqrt{2\Omega_k^{(n)}(t)}} e^{-i\int_{t_o}^{t}\Omega_k^{(n)}(t')\,dt'} \tag{3.71}$$

is iteratively defined by

$$\begin{aligned} (\Omega_k^{(0)})^2 &:= \omega_k^2 = \frac{E(k)}{a^2} + \mu^2 \\ (\Omega_k^{(n+1)})^2 &= \omega_k^2 - \frac{3}{4}\left(\frac{\dot{a}}{a}\right)^2 - \frac{3}{2}\frac{\ddot{a}}{a} + \frac{3}{4}\left(\frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}}\right)^2 - \frac{1}{2}\frac{\ddot{\Omega}_k^{(n)}}{\Omega_k^{(n)}}. \end{aligned} \tag{3.72}$$

Remarks:

1. (3.71), (3.72) is an iterative solution to (3.59). If $a(t) = const.$ one obtains the ultrastatic groundstate. The iteration procedure may break down yielding negative values for $(\Omega_k^{(n+1)})^2$. But one can show [41] that for a finite time interval and sufficiently large k $\Omega_k^{(n)}$ is always strictly positive. $\Omega_k^{(n)}$ can then be continued (smoothly in t) to *all* values of k.

2. Condition (3.69) (resp. (3.67)) is automatically satisfied by the Ansatz (3.71).

3. An adiabatic vacuum state depends on

   - the choice of initial time t in (3.70),
   - the order of iteration n,
   - the extrapolation of $\Omega_k^{(n)}$ to small values of k.

Lüders and Roberts [41] show that all adiabatic vacuum states are locally quasiequivalent. To this end, they consider a Bogoliubov transformation between two Fock states parametrized by functions $(q(k), p(k))$ resp. $(q'(k), p'(k))$

$$\begin{aligned} q'(k) &= \alpha(k)q(k) + \beta(k)\overline{q(k)}, \\ p'(k) &= \alpha(k)p(k) + \beta(k)\overline{p(k)}, \end{aligned} \tag{3.73}$$

where the Bogoliubov coefficients α and β have to satisfy

$$|\alpha(k)|^2 - |\beta(k)|^2 = 1.$$

Using (3.67) one can solve for β and gets

$$\beta(k) = -i(p'(k)q(k) - q'(k)p(k)). \tag{3.74}$$

The property of quasiequivalence of two such Fock states now depends on the asymptotic behaviour of $\beta(k)$. On the way to their main result they prove a necessary condition for quasiequivalence which we state (only for the case of the closed universe) for later reference:

Lemma 3.20 ([41], p.47) *If two Fock states (parametrized by functions $(q(k), p(k))$ resp. $(q'(k), p'(k))$) of the Klein-Gordon quantum field on the closed universe are locally quasiequivalent then*

$$\sum_{k=0}^{\infty}(k+1)^2|\beta(k)|^2 < \infty. \tag{3.75}$$

The main result of [41] now reads:

Theorem 3.21 (Theorems 3.3 and 5.7 of [41]) *a) In a closed Robertson-Walker spacetime any two adiabatic vacuum states are unitarily equivalent.*
b) In an open Robertson-Walker spacetime any two adiabatic vacuum states of iteration order $n \geq 1$ are locally quasiequivalent.
c) If ω is an adiabatic vacuum state on an open Robertson-Walker spacetime then $\pi_\omega|_{\mathcal{O}}$ is a factor when $\mathcal{O} = D(\mathcal{C})$ and $\mathcal{C}$ is an open bounded subset of some Σ_t with smooth boundary.

Thus, the class of adiabatic vacuum states satisfies the principle of local definiteness. Furthermore, for these states the expectation value of the energy-momentum tensor can be constructed using an adiabatic regularization procedure due to Parker and Fulling [47]. So the adiabatic vacua seem to be as good a class of physical states as the class of Hadamard states, and naturally the question arises what the connection between Hadamard states and adiabatic vacua might be.
Najmi and Ottewill [44] show that a Hadamard state on a Robertson-Walker space with flat spatial sections ($\kappa = 0$) has the same asymptotic behaviour in momentum space as an adiabatic vacuum state of order 0. Bernard [4] computes the high energy behaviour of Hadamard states on a Bianchi type-I spacetime and finds it in agreement with that of an adiabatic vacuum state of order 2. In [43] it is shown that the anticommutator function of certain states which are constructed by a WKB-expansion very similar to (3.71), (3.72) has Hadamard singularities. These results led Lüders and Roberts [41] to conjecture that Hadamard states and adiabatic vacua define the *same* class of physical states. Pirk [48] claims to have proven that in a spatially flat Robertson-Walker spacetime an adiabatic vacuum state is an Hadamard state if and only if it is of infinite order. The if-part of his "proof" is – to say the least – not trustworthy since he does not control convergence of infinite series and there is a priori no reason that an iteration like (3.72) will converge, the only-if-part is certainly false as we will see in a moment.
Now we formulate the first main physical result of this work in the following theorem:

Theorem 3.22 *The adiabatic vacuum states of order $n \in \mathbf{N}_o$ of a linear Klein-Gordon quantum field (3.57) on the Robertson-Walker spacetimes (3.53) are Hadamard states.*

Before we prove the theorem we state an immediate consequence:

Corollary 3.23 *All Hadamard states and adiabatic vacuum states of a linear Klein-Gordon quantum field on the Robertson-Walker spacetimes lie in the same local primary folium (quasiequivalence class) of states. (This also extends the validity of Theorem 3.21 to the case of the adiabatic vacuum of order 0 on the open Robertson-Walker spaces.)*

PROOF of Theorem 3.22:
The idea is again to compute the wavefront set of the two-point function of an n-th order adiabatic vacuum state. Starting with (3.65), (3.66) and inserting Definition 3.19 we obtain for the two-point function:

$$
\begin{aligned}
\Lambda_n^{(2)}(f_1, f_2) &= \lambda_n^{(2)}\left(\begin{pmatrix}\rho_o E f_1 \\ a^3\rho_1 E f_1\end{pmatrix}, \begin{pmatrix}\rho_o E f_2 \\ a^3\rho_1 E f_2\end{pmatrix}\right) \\
&= \int d\mu(\vec{k}) \left\langle \overline{\begin{pmatrix}\rho_o \widetilde{Ef_1} \\ a^3\rho_1 \widetilde{Ef_1}\end{pmatrix}}, \begin{pmatrix} a^6|\dot{T}_k^{(n)}|^2 & -a^3 T_k^{(n)}\overline{\dot{T}_k^{(n)}} \\ -a^3 \overline{T_k^{(n)}}\dot{T}_k^{(n)} & |T_k^{(n)}|^2 \end{pmatrix} \begin{pmatrix}\rho_o \widetilde{Ef_2} \\ a^3\rho_1 \widetilde{Ef_2}\end{pmatrix}\right\rangle,
\end{aligned}
$$

for $f_1, f_2 \in \mathcal{D}(\mathcal{M})$, where $T_k^{(n)}(t)$ denotes the solution of (3.59) with initial conditions (3.70). We use the orthogonality relation $(\phi_{\vec{k}}, \phi_{\vec{l}})_{L^2(\Sigma)} = \delta(\vec{k}, \vec{l})$ where δ is the delta function w.r.t. the measure $d\mu(\vec{k})$:

$$
\begin{aligned}
\Lambda_n^{(2)}(f_1, f_2) &= a^3 \int d\mu(\vec{k}) \int d\mu(\vec{l})\, \delta(\vec{k}, \vec{l}) \left\langle \overline{\begin{pmatrix}\rho_o(\widetilde{Ef_1})(\vec{k}) \\ \rho_1(\widetilde{Ef_1})(\vec{k})\end{pmatrix}}, \begin{pmatrix} a^3\overline{\dot{T}_k^{(n)}}\dot{T}_l^{(n)} & -a^3\overline{\dot{T}_k^{(n)}}T_l^{(n)} \\ -a^3\overline{T_k^{(n)}}\dot{T}_l^{(n)} & a^3\overline{T_k^{(n)}}T_l^{(n)} \end{pmatrix} \right. \\
&\qquad \left. \begin{pmatrix}\rho_o(\widetilde{Ef_2})(\vec{l}) \\ \rho_1(\widetilde{Ef_2})(\vec{l})\end{pmatrix}\right\rangle \\
&= a^3 \int_\Sigma d^3\sigma_y \int d\mu(\vec{k}) \int d\mu(\vec{l})\, \overline{\phi_{\vec{k}}(\vec{y})(\widetilde{Ef_1})(t, \vec{k})} \Big[a^3\overline{\dot{T}_k^{(n)}}\dot{T}_l^{(n)} - \overleftarrow{\partial_t}\, a^3\overline{T_k^{(n)}}\dot{T}_l^{(n)} \\
&\qquad -a^3\overline{\dot{T}_k^{(n)}}T_l^{(n)}\, \overrightarrow{\partial_t} + \overleftarrow{\partial_t}\, a^3\overline{T_k^{(n)}}T_l^{(n)}\, \overrightarrow{\partial_t}\Big] (\widetilde{Ef_2})(t, \vec{l})\phi_{\vec{l}}(\vec{y}) = \\
&= \int_{\Sigma_t} d^3y\sqrt{|h(t, \vec{y})|}\, \overline{\left[\int d\mu(\vec{k})\phi_{\vec{k}}(\vec{y})(\widetilde{Ef_1})(t, \vec{k}) \left(\frac{\dot{T}_k^{(n)}}{T_k^{(n)}} - \overleftarrow{\partial_t}\right)\right]} \\
&\qquad \cdot \left[\int d\mu(\vec{l}) a^3 |T_l^{(n)}|^2 \left(\frac{\dot{T}_l^{(n)}}{T_l^{(n)}} - \overrightarrow{\partial_t}\right) (\widetilde{Ef_2})(t, \vec{l})\phi_{\vec{l}}(\vec{y})\right].
\end{aligned}
$$

Finally, noting that $E' = -E$, we can abbreviate the result in the form

$$
\begin{aligned}
\Lambda_n^{(2)}(f_1, f_2) &= (P_n E f_1, A_n P_n E f_2)_{L^2(\Sigma_t)} \text{ or} \\
\Lambda_n^{(2)}(x_1, x_2) &= -\int_{\Sigma_t} d^3y\sqrt{|h(t, \vec{y})|}\, \overline{E(x_1; t, \vec{y})\, \overleftarrow{P_n}} A_n\, \overrightarrow{P_n}\, E(t, \vec{y}; x_2),
\end{aligned} \tag{3.76}
$$

where[2] A_n, P_n shall denote the operators

$$
(A_n f)(t, \vec{y}) := \int d\mu(\vec{k}) a^3(t) |T_k^{(n)}(t)|^2 \tilde{f}(t, \vec{k})\phi_{\vec{k}}(\vec{y})
$$

[2]Remember that (3.76) is a somewhat sloppy notation. The product of the two distributions is properly defined by localization around Σ_t and convolution of the Fourier transforms as in (2.27) or (3.39). This is the reason why one has to know $T_k^{(n)}(t)$ in a whole (infinitesimal) neighborhood of Σ_t.

$$
\begin{aligned}
(P_n f)(t,\vec{y}) &:= (B_n(t)-\partial_t)f(t,\vec{y}) \\
(B_n f)(t,\vec{y}) &:= \int d\mu(\vec{k})\frac{\dot{T}_k^{(n)}}{T_k^{(n)}}\tilde{f}(t,\vec{k})\phi_{\vec{k}}(\vec{y}) \\
\tilde{f}(t,\vec{k}) &= \int_\Sigma d^3\sigma_z\,\overline{\phi_{\vec{k}}(\vec{z})}f(t,\vec{z}) \text{ for } f\in\mathcal{C}^\infty(\mathcal{M}).
\end{aligned}
\tag{3.77}
$$

We recognize with satisfaction that the two-point function (3.76) is exactly of the form (3.42) treated in connection with the ultrastatic ground state, therefore we can apply Theorem 3.15 if we make sure that the operators A_n and P_n satisfy the sufficient conditions of this theorem. So we have to investigate the properties of $|T_k^{(n)}(t)|^2$ and $\frac{\dot{T}_k^{(n)}}{T_k^{(n)}}$ as operators. By the defining equ. (3.70),

$$
\begin{aligned}
a_n(t,k) &:= |T_k^{(n)}(t)|^2 = (a^3 2\Omega_k^{(n)}(t))^{-1} \\
b_n(t,k) &:= \frac{\dot{T}_k^{(n)}(t)}{T_k^{(n)}(t)} = -\frac{3}{2}\frac{\dot{a}(t)}{a(t)} - \frac{1}{2}\frac{\dot{\Omega}_k^{(n)}(t)}{\Omega_k^{(n)}(t)} - i\Omega_k^{(n)}(t)
\end{aligned}
\tag{3.78}
$$

on a hypersurface Σ_t. Since $T_k^{(n)}(t)$ is a solution of equation (3.59) we have (leaving for a moment the k's and n's away)

$$
\begin{aligned}
\left(-\partial_t - 3\frac{\dot{a}}{a} - \frac{\dot{T}}{T}\right)\left(\frac{\dot{T}}{T}-\partial_t\right) &= -\frac{\ddot{T}}{T} + \frac{\dot{T}^2}{T^2} - \frac{\dot{T}}{T}\partial_t + \partial_t^2 - 3\frac{\dot{a}}{a}\frac{\dot{T}}{T} + 3\frac{\dot{a}}{a}\partial_t - \frac{\dot{T}^2}{T^2} + \frac{\dot{T}}{T}\partial_t \\
&= \partial_t^2 + 3\frac{\dot{a}}{a}\partial_t - \frac{1}{T}(\ddot{T} + 3\frac{\dot{a}}{a}\dot{T}) \\
&= \partial_t^2 + 3\frac{\dot{a}}{a}\partial_t + \omega^2 \\
&= \Box_g + \mu^2,
\end{aligned}
$$

hence the operator Q of Theorem 3.15 reads in this case

$$
\begin{aligned}
(Q_n f)(t,\vec{y}) &= \int d\mu(\vec{k})\, q_n(t,k)\tilde{f}(t,\vec{k})\phi_{\vec{k}}(\vec{y}) \\
q_n(t,k) &= \partial_t + 3\frac{\dot{a}}{a} + \frac{\dot{T}_k^{(n)}}{T_k^{(n)}} \\
&= \partial_t + \frac{3}{2}\frac{\dot{a}}{a} - \frac{1}{2}\frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}} - i\Omega_k^{(n)}.
\end{aligned}
\tag{3.79}
$$

We summarize the properties of A_n, B_n and Q_n in a lemma:

Lemma 3.24 *For all* $n\in\mathbf{N}_o$*:*
i) $A_n(t)\in L^{-1}_{1,0}$*, it is an elliptic pseudodifferential operator.*
ii) $B_n(t)\in L^1_{1,0}$*.*
iii) $Q_n(t)\in L^1_{1,0}$ *with principal symbol* $q(t;\xi)$ *such that* $q^{-1}(0)\setminus\{0\}\subset\{(x,\xi)\in T^*\mathcal{M};\ \xi_0>0\}$*.*

PROOF:
Looking at the iterative definition (3.72) of $\Omega_k^{(n)}(t)$ and noting that

$$
\begin{aligned}
\dot{\omega}_k &= \frac{\dot{a}}{a}\frac{\mu^2-\omega_k^2}{2\omega_k} \\
\ddot{\omega}_k &= \left(\frac{\dot{a}}{a}\right)^2\frac{\mu^4+2\mu^2\omega_k^2-3\omega_k^4}{4\omega_k^3} + \frac{\ddot{a}}{a}\frac{\mu^2-\omega_k^2}{2\omega_k} \quad \text{etc.}
\end{aligned}
$$

we see that $\Omega_k^{(n)}$ and $\dot{\Omega}_k^{(n)}/\Omega_k^{(n)}$ depend on k only as rational functions of $\omega_k = (E(k)/a^2 + \mu^2)^{1/2}$. The analysis of the asymptotic behaviour of these functions has been carried out by Lüders and Roberts [41]. From their work one can conclude that

$$\begin{aligned} \frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}} &\in S^0_{1,0} \\ \Omega_k^{(n)} &\in S^1_{1,0} \text{ with leading term } \omega_k \end{aligned} \tag{3.80}$$

(for all $n \in \mathbf{N}_o$ and always uniformly on a bounded interval in t). Therefore, for $\kappa = 0$ (in which case $\phi_{\vec{k}}(\vec{y}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{y}}$), the lemma is proven, whereas for $\kappa = \pm 1$ it remains to be shown that A_n, B_n, Q_n are indeed pseudodifferential operators.
Let us consider as a prototype

$$(Df)(t,\vec{y}) := \int d\mu(\vec{k})\, \omega_k(t) \tilde{f}(t,\vec{k}) \phi_{\vec{k}}(\vec{y}).$$

Localizing in a coordinate neighborhood around $\vec{y} \in \Sigma_t$ and denoting the Fourier transform (w.r.t. $e^{i\vec{y}\vec{\xi}}$) of f by $\hat{f}$ we have

$$\begin{aligned} (Df)(t,\vec{y}) &= \int d\mu(\vec{k})\, \omega_k(t)\phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, \overline{\phi_{\vec{k}}(\vec{z})} f(t,\vec{z}) \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} d^3\xi\, \hat{f}(t,\vec{\xi}) \int d\mu(\vec{k})\, \omega_k(t)\phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, e^{i\vec{z}\vec{\xi}}\overline{\phi_{\vec{k}}(\vec{z})} \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} d^3\xi\, \hat{f}(t,\vec{\xi}) e^{i\vec{y}\vec{\xi}} \left\{ e^{-i\vec{y}\vec{\xi}} \int d\mu(\vec{k})\, \omega_k(t)\phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, \overline{\phi_{\vec{k}}(\vec{z})} e^{i\vec{z}\vec{\xi}} \right\} \\ &=: \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} d^3\xi\, \hat{f}(t,\vec{\xi}) e^{i\vec{y}\vec{\xi}} d(t,\vec{y},\vec{\xi}). \end{aligned}$$

This is a pseudodifferential operator if $d(t,\vec{y},\vec{\xi})$ is a symbol. Using the fact that the $\phi_{\vec{k}}(\vec{y})$ are a complete set of eigenfunctions of the Laplace-Beltrami operator (3.58) on Σ_t (which is selfadjoint w.r.t. $d^3\sigma_z$) we obtain

$$\begin{aligned} d(t,\vec{y},\vec{\xi}) &= e^{-i\vec{y}\vec{\xi}} \int d\mu(\vec{k})\, \omega_k(t)\phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, \overline{\phi_{\vec{k}}(\vec{z})} e^{i\vec{z}\vec{\xi}} \\ &= e^{-i\vec{y}\vec{\xi}} \int d\mu(\vec{k})\, \phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, (-{}^{(3)}\Delta_z + \mu^2)^{1/2} \overline{\phi_{\vec{k}}(\vec{z})} e^{i\vec{z}\vec{\xi}} \\ &= e^{-i\vec{y}\vec{\xi}} \int d\mu(\vec{k})\, \phi_{\vec{k}}(\vec{y}) \int_\Sigma d^3\sigma_z\, \overline{\phi_{\vec{k}}(\vec{z})} (-{}^{(3)}\Delta_z + \mu^2)^{1/2} e^{i\vec{z}\vec{\xi}} \\ &= e^{-i\vec{y}\vec{\xi}} (-{}^{(3)}\Delta_y + \mu^2)^{1/2} e^{i\vec{y}\vec{\xi}} \\ &= \left\{ \frac{|\vec{\xi}|^2}{a^2} \left[1 - \kappa \left(\frac{\vec{y}\vec{\xi}}{\xi} \right)^2 \right] + i\frac{|\vec{\xi}|}{a^2} 3\kappa \frac{\vec{y}\vec{\xi}}{\xi} + \mu^2 \right\}^{1/2}, \end{aligned}$$

which is a symbol of order 1 (note that $|\vec{y}| < 1$ for $\kappa = +1$), and consequently $D \in L^1_{1,0}(\Sigma_t)$. A principal symbol of D is given by

$$\frac{|\vec{\xi}|}{a} \left[1 - \kappa \left(\vec{y}\vec{\xi}/\xi \right)^2 \right]^{1/2}.$$

Now the lemma follows when we remember that a_n and b_n are rational expressions in ω_k with leading terms $(a^3 2\omega_k)^{-1}$ resp. $-i\omega_k$ and the correct asymptotic properties (3.80). $\square$

Applying Theorem 3.15 we can conclude that (3.76) has indeed wavefront set of an Hadamard state for all $n \in \mathbf{N}_o$. This proves the theorem. $\square$

Remark:

There are no obvious obstacles to extending our analysis to spacetimes which are homogeneous, but not necessarily isotropic (like the Bianchi-I-spacetime), or to the case of a Klein-Gordon field coupled to the scalar curvature, i.e. a field equation of the form

$$(\Box_g + \mu^2 + \xi R)\Phi = 0.$$

3.5 A counterexample

The states we have presented in sections 3.3 and 3.4 are constructed on very special spacetimes: in the one case the spacetime possesses a static Killing vectorfield, in the other there exists a preferred foliation of the spacetime into homogeneous Cauchy surfaces such that the wave equation separates into time- and space-dependent parts. It immediately arises the question whether physical states can also be constructed on arbitrarily curved globally hyperbolic spacetimes. Before we give our own solution of this problem (in the next section) let us investigate two proposals existing in the literature for such a general construction, namely the method of "Hamiltonian diagonalization" (see the references in [20]) and the construction of "energy states" [3, 9]. Instead of presenting these constructions in detail we want to pick out one particular example of a state that lies in both classes and show that this state is in general physically *not* acceptable.

Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime possessing a complete Cauchy surface Σ (with volume element $d^3\sigma$) and $A := \overline{-\Delta + \mu^2}$ the (closure of the) Laplace-Beltrami operator on Σ (with $\mu > 0$). Let (Γ, σ) be the phase space of initial data of the Klein-Gordon field on Σ (equ. (3.28)). The idea is to mimic the construction (3.29) of the ultrastatic groundstate w.r.t. the Cauchy surface Σ, i.e. we define a one-particle Hilbertspace structure on Γ by

$$\begin{aligned} k^\Sigma : \Gamma &\rightarrow \mathcal{H} := L^2_{\mathbf{C}}(\Sigma, d^3\sigma) \\ (f, p) &\mapsto \frac{1}{\sqrt{2}}(A^{1/4} f - i A^{-1/4} p). \end{aligned} \tag{3.81}$$

Of course, since A depends on the chosen Cauchy surface each choice of Σ yields a different state, nevertheless (3.81) is a well defined one-particle Hilbertspace structure and therefore defines an (in general not stationary) quasifree state of the Klein-Gordon quantum field on $(\mathcal{M}, g)$. So straightforward this construction may appear, it does in general not yield reasonable physical states. To show this we put the state (3.81) on a closed Robertson-Walker spacetime and prove that it does not lie in the folium of an Hadamard state:

Theorem 3.25 *Let $(\mathcal{M}^+, g)$ be the closed Robertson-Walker spacetime (3.53) ($\kappa = +1$), Σ_t a homogeneous Cauchy surface of $\mathcal{M}^+$ and ω_t the quasifree state of the Klein-Gordon quantum*

field defined by k^{Σ_t} (equ. (3.81)).
Then, ω_t is not quasiequivalent to an Hadamard state.

PROOF:
The two-point function of (3.81) reads

$$
\begin{aligned}
\lambda^{(2)}(F_1, F_2) &= \frac{1}{2}\langle (A^{1/2} f_1 - i p_1), (f_2 - i A^{-1/2} p_2)\rangle_{\mathcal{H}^t} \\
&= \frac{1}{2}\langle F_1, \begin{pmatrix} A^{1/2} & -i \\ i & A^{-1/2} \end{pmatrix} F_2 \rangle_{\mathcal{H}^t} \\
&= \frac{1}{2}\left\langle \begin{pmatrix} f_1 \\ a^3 p_1 \end{pmatrix}, \begin{pmatrix} A^{1/2} & -\frac{i}{a^3} \\ \frac{i}{a^3} & \frac{1}{a^6} A^{-1/2} \end{pmatrix} \begin{pmatrix} f_2 \\ a^3 p_2 \end{pmatrix} \right\rangle_{\mathcal{H}^t} \\
&= \frac{1}{2}\int d\mu(\vec{k}) \left\langle \overline{\begin{pmatrix} \tilde{f}_1 \\ a^3 \tilde{p}_1 \end{pmatrix}}, \begin{pmatrix} \omega_k & -\frac{i}{a^3} \\ \frac{i}{a^3} & \frac{1}{a^6 \omega_k} \end{pmatrix} \begin{pmatrix} \tilde{f}_2 \\ a^3 \tilde{p}_2 \end{pmatrix} \right\rangle, \qquad (3.82)
\end{aligned}
$$

where $f_i, p_i \in \mathcal{C}_o^\infty(\Sigma_t)$, $\mathcal{H}^t := L^2_{\mathbb{C}}(\Sigma_t, d^3\sigma)$, $\omega_k(t)$ is given by (3.60) and the (generalized) Fourier transform by (3.63). (3.82) is of the form (3.65), (3.66) of a homogeneous, isotropic Fock state with $p(k) := \sqrt{\omega_k(t)/2}$, $q(k) := i(a^3\sqrt{2\omega_k(t)})^{-1}$.
Let us compare this with the adiabatic vacuum state of order 0 (Definition 3.19), where

$$
\begin{aligned}
q^{(0)}(k) &= W_k^{(0)}(t) = a^{-3/2}(2\omega_k)^{-1/2} e^{-i\int_{t_o}^t \omega_k(t')\,dt'} \\
p^{(0)}(k) &= a^3 \dot{W}_k^{(0)}(t) = -a^3 \left[i\omega_k + \frac{\dot{a}}{a} + \frac{\dot{a}}{a}\frac{\mu^2}{2\omega_k^2} \right] W_k^{(0)}(t),
\end{aligned}
$$

and compute the Bogoliubov coefficient $\beta(k)$ between these two states according to equ. (3.74):

$$
|\beta(k)| = \frac{1}{2\omega_k}\frac{1}{a^{3/2}}\left|\frac{\dot{a}}{a}\right|\left[1 + \frac{\mu^2}{2\omega_k^2}\right].
$$

Now, since $\omega_k^2 = k(k+2)/a^2 + \mu^2$, we observe that

$$
\sum_{k=0}^{\infty} |\beta(k)|^2 (k+1)^2 = \infty,
$$

for $\dot{a} \neq 0$, therefore, by Lemma 3.20, these two states cannot be quasiequivalent. Since the adiabatic vacuum state of order 0 is an Hadamard state (Theorem 3.22) our state (3.81) does not lie in the folium of Hadamard states. □

Remark:
Of course, on certain spacetimes (e.g. the ultrastatic spacetimes, as we have seen in section 3.3) (3.81) may be a well behaved Hadamard state. The point we want to make here is just that the seemingly very elegant and general construction of (3.81) (and similar ones existing in the literature) does *in general* (on an arbitrarily curved spacetime) not lead to a physical state.
Let us remark that this counterexample does not come as a surprise, it only confirms the criticism already raised by Fulling [20] against the method of Hamiltonian diagonalization (where states are constructed by selecting ad hoc the positive frequencies on a single Cauchy surface as in our example), which also applies to the states constructed in [3] and [9].

3.6 Construction of Hadamard states

We learnt from the example in the last section that the "positive frequencies" in a non-stationary spacetime cannot be fixed on a Cauchy surface, but must be dynamically determined off the Cauchy surface. We saw in the proofs of Theorems 3.15 and 3.22 that this is achieved by a separation of the Klein-Gordon operator into first-order factors that project out the correct positive frequencies from the fundamental solution in an (infinitesimal) neighborhood of the Cauchy surface. This was trivial in the ultrastatic case where the Laplace-Beltrami operator is time-independent. In the case of the adiabatic vacua an exact factorization of the wave operator was accomplished by separating off the time dependence, using a solution of the ordinary differential equation (3.59) and imposing initial conditions that enforce the correct asymptotic behaviour.

On an arbitrarily curved globally hyperbolic spacetime such a method is no longer possible. In this section we will present a general technique for constructing Hadamard states by a local factorization of the wave operator with the help of pseudodifferential operators.

First we give a clever parametrization of Fock states due to Deutsch and Najmi [11]:

Theorem 3.26 *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime with Cauchy surface Σ. Let (Γ, σ) be the phase space of initial data on Σ of the Klein-Gordon field (see section 3.1). Let R be a symmetric and I a symmetric, positive and invertible operator on $L^2_{\mathbf{R}}(\Sigma, d^3\sigma)$. Then, with $\mathcal{H} = L^2_{\mathbf{C}}(\Sigma, d^3\sigma)$,*

$$\begin{aligned} k^\Sigma : \Gamma &\to \mathcal{H} \\ (f,p) &\mapsto (2I)^{-1/2}\left[(R - iI)f - p\right] \end{aligned} \tag{3.83}$$

is a one-particle Hilbertspace structure and defines a Fock state.

PROOF:
For $F_i = (f_i, p_i) \in \Gamma,\ i = 1, 2,$

$$\begin{aligned} 2\mathrm{Im}\langle k^\Sigma F_1, k^\Sigma F_2\rangle_{\mathcal{H}} &= \mathrm{Im}\langle (R - iI)f_1 - p_1, I^{-1}\left[(R - iI)f_2 - p_2\right]\rangle_{\mathcal{H}} \\ &= \langle If_1, I^{-1}(Rf_2 - p_2)\rangle_{\mathcal{H}} - \langle Rf_1 - p_1, f_2\rangle_{\mathcal{H}} \\ &= -\langle f_1, p_2\rangle_{\mathcal{H}} + \langle p_1, f_2\rangle_{\mathcal{H}} \\ &= \sigma(F_1, F_2), \\ 2\mathrm{Re}\langle k^\Sigma F_1, k^\Sigma F_2\rangle_{\mathcal{H}} &= \langle (Rf_1 - p_1), I^{-1}(Rf_2 - p_2)\rangle_{\mathcal{H}} + \langle If_1, f_2\rangle_{\mathcal{H}} \\ &= \langle (Rf_1 - p_1), I^{-1}(Rf_2 - p_2)\rangle_{\mathcal{H}} + \langle f_1, If_2\rangle_{\mathcal{H}} \\ &=: 2\mu(F_1, F_2). \end{aligned}$$

μ is a scalar product since I is positive and symmetric. (3.11) is automatically satisfied because

$$\begin{aligned} |\mathrm{Im}\langle u, v\rangle|^2 &\leq |\langle u, v\rangle|^2 \leq \langle u, u\rangle\langle v, v\rangle \\ &= (\mathrm{Re}\langle u, u\rangle + i\mathrm{Im}\langle u, u\rangle)(\mathrm{Re}\langle v, v\rangle + i\mathrm{Im}\langle v, v\rangle) \\ &= \mathrm{Re}\langle u, u\rangle\mathrm{Re}\langle v, v\rangle \end{aligned}$$

is fulfilled for any scalar product $\langle\cdot,\cdot\rangle$. Since $\mathcal{H}$ is the completion of $k^\Sigma\Gamma$, k^Σ describes a Fock state with one-particle Hilbertspace $\mathcal{H}$. □

As usual, we calculate the two-point function in the representation (3.83):

$$
\begin{aligned}
\Lambda_\Sigma^{(2)}(h_1,h_2) &= \langle k^\Sigma(\rho_o Eh_1,\rho_1 Eh_1), k^\Sigma(\rho_o Eh_2,\rho_1 Eh_2)\rangle_{\mathcal{H}} \\
&= \frac{1}{2}\left\langle I^{-1/2}\left[(R-iI)\rho_o Eh_1-\rho_1 Eh_1\right], I^{-1/2}\left[(R-iI)\rho_o Eh_2-\rho_1 Eh_2\right]\right\rangle_{\mathcal{H}} \\
&= \frac{1}{2}\left\langle (R-iI-n^\alpha\nabla_\alpha)Eh_1, I^{-1}(R-iI-n^\alpha\nabla_\alpha)Eh_2\right\rangle_{L^2_{\mathbf{C}}(\Sigma,d^3\sigma)}
\end{aligned}
\tag{3.84}
$$

for $h_i\in\mathcal{D}(\mathcal{M}),\ i=1,2$, where n^α is the unit-normalfield on Σ and E the fundamental solution of the Klein-Gordon equation in $(\mathcal{M},g)$. Comparing with the expressions (3.76)–(3.78) we note that (3.84) is of the same form as the two-point function of the adiabatic vacua even if $(\mathcal{M},g)$ is an arbitrary spacetime. With this simple representation of Fock states and the adiabatic vacua as a guiding example at hand we have now a clear picture of how one can construct Hadamard states on arbitrary curved spacetimes: we have to look for pseudodifferential operators R and I (with the properties stated in Theorem 3.26, and I elliptic) such that the Klein-Gordon operator $\Box_g+\mu^2$ can be factorized into $Q(R-iI-n^\alpha\nabla_\alpha)$ where Q is a pseudodifferential operator having the property stated in Theorem 3.15. Of course, in general we cannot expect to obtain such a factorization exactly, but locally it can always be arranged modulo "smoothing operators" in $L^{-\infty}(\Sigma)$. This is sufficient for our argument in the proof of Theorem 3.15 as the following little lemma shows:

Lemma 3.27 *Let $R_1,R_2\in L^{-\infty}(\Sigma)$.*
Then $(R_1 n^\alpha\nabla_\alpha+R_2)E$ is smooth.

PROOF:
Let us take a local coordinate system $X\subset\mathcal{M}$, where Σ is given by $x^0=0$ and let $R:=R_1\partial/\partial x^0+R_2$.
We write

$$RE=R\chi(D)E+R(1-\chi(D))E \tag{3.85}$$

where $\chi(\xi)\in S^0_{1,0}(\mathbf{R}^4)$ has support only in a small conic neighborhood of the ξ_0-axis where no singular direction of E lies and $\chi=1$ at infinity in a second, smaller conic neighborhood, and $\chi(D)$ denotes the pseudodifferential operator with symbol $\chi(\xi)$.
Then $R\chi(D)$ and $R(1-\chi(D))$ are 4-dim. pseudodifferential operators and we can apply Theorem 2.23 to calculate the wavefront set of (3.85). The first term is smooth since no singular directions of $R\chi(D)$ and E coincide, the second term is smooth since $R(1-\chi(D))\in L^{-\infty}(X)$ (and $WF_{\mathcal{M}}(E)=\emptyset$ as we have seen in the proof of Lemma 3.14). $\Box$

For the following let us fix a spacelike Cauchy surface Σ of $(\mathcal{M},g)$ with induced metric h_{ij} and unit-normalfield n^α. For reasons of notational simplicity we work in **Gaußian normal coordinates** in a neighborhood of Σ, i.e. we choose a local coordinate patch $S\subset\Sigma$ and consider for each point $p=(x^1,x^2,x^3)\in S$ the geodesic that starts from p with tangent $\pm n^\alpha$. Then, each point in the neighborhood of S can be labeled by (t,x^1,x^2,x^3) where t is the proper time along the geodesic on which it lies ($t<(>)0$ for points that lie before (after) Σ). The geodesics may cross after some time, but for each S there is certainly a finite interval $[-T,T]$

in which the such constructed Gaußian normal coordinates are well defined (for details see [59, p.42]). The hypersurface S is then given by $t=0$, the metric g reads in these coordinates

$$g_{\mu\nu} = \begin{pmatrix} 1 & \\ & -h_{ij}(t,\vec{x}) \end{pmatrix}$$

and the Klein-Gordon operator reduces to

$$\begin{aligned} P \equiv \Box_g + \mu^2 &= \frac{1}{\sqrt{|g|}}\partial_\mu(\sqrt{|g|}g^{\mu\nu}\partial_\nu\cdot) + \mu^2 \\ &= \partial_t^2 + K(t,\vec{x})\partial_t -^{(3)}\Delta_h + \mu^2 \\ &= \frac{1}{\sqrt{h}}\partial_t(\sqrt{h}\partial_t\cdot) - \frac{1}{\sqrt{h}}\partial_i(\sqrt{h}h^{ij}\partial_j\cdot) + \mu^2, \end{aligned} \tag{3.86}$$

where ${}^{(3)}\Delta_h$ is the (time-dependent) Laplace-Beltrami operator on S and

$$K(t,\vec{x}) = \partial_t \ln\sqrt{h} = \nabla_\alpha n^\alpha = g^{\alpha\beta}K_{\alpha\beta}$$

is the trace of the extrinsic curvature $K_{\alpha\beta}$ of the hypersurface $t = const$.
In what follows we use the **notation** $a(t,x,D)$ for the pseudodifferential operator with symbol $a(t,x,\xi)$, we write $a(t,x,\xi) \in S^m$ if $a(t,x,\xi)$ and $\partial_t^l a(t,x,\xi) \in S^m_{1,0}(S \times \mathbf{R}^3), l = 1,2,\ldots,$ uniformly in $t \in [-T,T]$ (similarly $a(t,x,D) \in L^m$), and here is always $x \in S, \xi \in \mathbf{R}^3$ and $t \in [-T,T]$.
We want to factorize (3.86) into

$$P = P_1 \circ P_2 - r_1(t) \text{ on } [-T,T]$$

with $r_1(t) \in L^{-\infty}$. The principal symbol of P is

$$p(t,x,\tau,\xi) := -\tau^2 + h^{kl}(t,x)\xi_k\xi_l$$

and its characteristic roots $\tau_\pm$ are given by

$$p(t,x,\tau_\pm,\xi) = 0 \Leftrightarrow \tau_\pm = \pm\lambda(t,x,\xi) := \pm\left(h^{kl}(t,x)\xi_k\xi_l\right)^{1/2} \in S^1. \tag{3.87}$$

It follows

$$|\lambda(t,x,\xi)| = \left(h^{kl}\xi_k\xi_l\right)^{1/2} \geq C|\xi| \text{ for } |\xi| \geq M \tag{3.88}$$

for some positive constants C and M. Let us modify the symbol $(h^{kl}\xi_k\xi_l)^{1/2}$ for $|\xi| < M$ such that $|\lambda(t,x,\xi)| \geq \epsilon > 0$ (by Lemma 2.2d), this changes λ only modulo $S^{-\infty}$). We make the Ansatz

$$\begin{aligned} P_1 &= -a(t,x,D) - \frac{1}{\sqrt{h}}\partial_t\sqrt{h} \\ P_2 &= a(t,x,D) - \partial_t \end{aligned} \tag{3.89}$$

and determine a by an asymptotic expansion of its symbol:

$$\begin{aligned} a^{(n)}(t,x,\xi) &:= \sum_{\nu=0}^{n} b^{(\nu)}(t,x,\xi) \\ P_1^{(n)} &:= -a^{(n)}(t,x,D) - \frac{1}{\sqrt{h}}\partial_t\sqrt{h} \\ P_2^{(n)} &:= a^{(n)}(t,x,D) - \partial_t, \end{aligned} \tag{3.90}$$

where $b^{(\nu)}$ shall denote symbols in $S^{1-\nu}$.
For $\mathbf{n = 0}$ we set

$$b^{(0)}(t,x,\xi) := -i\lambda(t,x,\xi) \quad \in S^1. \tag{3.91}$$

Then the principal symbol of $P_1 \circ P_2 - P$ is

$$\lambda^2 - \tau\lambda + \lambda\tau - \tau^2 - (-\tau^2 + h^{kl}\xi_k\xi_l) = 0 \; (mod\, S^1),$$

i.e. we have

$$P_1^{(0)} \circ P_2^{(0)} - P = r_1^{(0)}(t,x,D) \text{ on } [-T,T]$$

with $r_1^{(0)} \in L^1$ ($r_1^{(0)}(t,x,\xi)$ is an infinite asymptotic sum deriving from the asymptotic expansion (2.11) of the product $\lambda(t,x,D) \circ \lambda(t,x,D)$ which we do not want to give here).
Let us now iterate **from n to n+1** by assuming that $b^{(\nu)}(t,x,\xi), \nu \le n$, are already determined such that

$$P_1^{(n)} \circ P_2^{(n)} - P = r_1^{(n)}(t,x,D) \text{ on } [-T,T]$$

for some $r_1^{(n)} \in L^{1-n}$.
We set

$$b^{(n+1)}(t,x,\xi) := -\frac{i}{2}\frac{r_1^{(n)}(t,x,\xi)}{\lambda(t,x,\xi)} \quad \in S^{-n}. \tag{3.92}$$

This is well defined since we have modified λ at small values of ξ such that $\lambda \neq 0$, and $b^{(n+1)} \in S^{-n}$ because of (3.88) and the assumption on $r_1^{(n)}$. Then we have

$$\begin{aligned} P_1^{(n+1)} \circ P_2^{(n+1)} - P &= (P_1^{(n)} \circ P_2^{(n)} - P) - b^{(n+1)}(t,x,D)P_2^{(n)} \\ &\quad + P_1^{(n)} b^{(n+1)}(t,x,D) - b^{(n+1)}(t,x,D) b^{(n+1)}(t,x,D) \\ &= r_1^{(n)}(t,x,D) - b^{(n+1)}(t,x,D)(-i\lambda(t,x,D) - \partial_t) \\ &\quad + (i\lambda(t,x,D) - \frac{1}{\sqrt{h}}\partial_t\sqrt{h}) b^{(n+1)}(t,x,D) \; (mod\, L^{-n}) \end{aligned}$$

and the principal symbol of this expression is

$$\begin{aligned} & r_1^{(n)} - b^{(n+1)}(-i\lambda - i\tau) + (i\lambda - i\tau) b^{(n+1)} = \\ = \; & r_1^{(n)} + 2i\lambda b^{(n+1)} = 0 \; (mod\, S^{-n}), \end{aligned}$$

i.e. we have

$$P_1^{(n+1)} \circ P_2^{(n+1)} - P = r_1^{(n+1)}(t,x,D) \text{ on } [-T,T] \tag{3.93}$$

with $r_1^{(n+1)} \in L^{-n}$.
From Lemma 2.3 we can now conclude that

$$\begin{aligned} s(t,x,\xi) &\sim -\frac{1}{2i}\sum_{\nu=0}^{\infty}\left[b^{(\nu)}(t,x,\xi) - \overline{b^{(\nu)}(t,x,-\xi)}\right] \quad \in S^1 \\ r(t,x,\xi) &\sim \frac{1}{2}\sum_{\nu=0}^{\infty}\left[b^{(\nu)}(t,x,\xi) + \overline{b^{(\nu)}(t,x,-\xi)}\right] \quad \in S^0 \end{aligned} \tag{3.94}$$

define symbols ($mod\, S^{-\infty}$) in the specified classes. s has principal symbol

$$-\mathrm{Im}\, b^{(0)} = \lambda(t,x,\xi) = \left(h^{kl}(t,x)\xi_k\xi_l\right)^{1/2}$$

which is elliptic and positive. Since the principal symbol is the same for the adjoint (equ. (2.13)), we can modify s (smoothly in $t \in [-T, T]$) modulo $S^{-\infty}$ such that

$$I(t) := \frac{1}{2}\left[s(t,x,D) + s(t,x,D)^t\right] \tag{3.95}$$

is a strictly positive, elliptic, symmetric pseudodifferential operator in S^1 mapping real functions to real functions. Similarly, we define

$$R(t) := \frac{1}{2}\left[r(t,x,D) + r(t,x,D)^t\right] \quad \in S^0 \tag{3.96}$$

and claim that $I(t)$ and $R(t)$ realize via Theorem 3.26 a quasifree Hadamard state. In fact, comparing the two-point function (3.84) with the one (3.41) dealt with in Theorem 3.15, we see that we only have to prove that the operator $R - iI - \partial_t$ properly factorizes the wave operator: The two-point function (3.84) can be split into four terms

$$\begin{aligned}
\Lambda^{(2)}_\Sigma(h_1,h_2) &= \frac{1}{2}\left\langle (R - iI - \partial_t)Eh_1, I^{-1}(R - iI - \partial_t)Eh_2\right\rangle \\
&= \frac{1}{2}\left\langle \left[\frac{1}{2}(r + r^t - is - is^t) - \partial_t\right] Eh_1, I^{-1}\left[\frac{1}{2}(r + r^t - is - is^t) - \partial_t\right] Eh_2\right\rangle \\
&= \frac{1}{8}\Big\langle (r - is - \partial_t)Eh_1 + (r^t - is^t - \partial_t)Eh_1, \\
&\qquad\qquad I^{-1}\left[(r - is - \partial_t)Eh_2 + (r^t - is^t - \partial_t)Eh_2\right]\Big\rangle .
\end{aligned} \tag{3.97}$$

From equations (3.89)–(3.93) it follows after iteration

$$P_1(t) \circ P_2(t) = P + r_1(t,x,D) \text{ on } [-T,T]$$

where

$$\begin{aligned}
P_1(t) &= -a(t,x,D) - \frac{1}{\sqrt{h}}\partial_t\sqrt{h} \\
P_2(t) &= a(t,x,D) - \partial_t \\
a(t,x,\xi) &\sim \sum_{\nu=0}^{\infty} b^{(\nu)}(t,x,\xi) \sim r(t,x,\xi) - is(t,x,\xi) \\
r_1(t,x,D) &\in L^{-\infty},
\end{aligned}$$

and hence

$$(-r + is - \frac{1}{\sqrt{h}}\partial_t\sqrt{h})(r - is - \partial_t) = P + r_1 \text{ on } [-T,T].$$

By forming the adjoint one notes that this is equivalent to

$$\begin{aligned}
& -a \circ a - \frac{1}{\sqrt{h}}\partial_t\sqrt{h}a + a\partial_t = -\Delta + \mu^2 + r_1 \\
\Leftrightarrow\ & -a^t \circ a^t - \frac{1}{\sqrt{h}}\partial_t\sqrt{h}a^t + a^t\partial_t = -\Delta + \mu^2 + r_1^t \\
\Leftrightarrow\ & (-r^t + is^t - \frac{1}{\sqrt{h}}\partial_t\sqrt{h})(r^t - is^t - \partial_t) = P + r_1^t \text{ on } [-T,T]
\end{aligned}$$

with $r_1^t \in L^{-\infty}$. So let us define

$$Q_1 := -r + is - \frac{1}{\sqrt{h}}\partial_t\sqrt{h}, \quad Q_2 := -r^t + is^t - \frac{1}{\sqrt{h}}\partial_t\sqrt{h},$$

the principal symbol of both of them being

$$q(t,x,\xi_0,\xi) = i\lambda(t,x,\xi) - i\xi_0 = i\left(h^{kl}(t,x)\xi_k\xi_l\right)^{1/2} - i\xi_0,$$

i.e. $q^{-1}(0) \setminus \{0\} \subset \{(t,x;\xi_0,\xi) \in T^*([-T,T]\times S);\ \xi_0 > 0\}$, as desired for the application of Theorem 3.15. Since

$$\begin{aligned} Q_1(r - is - \partial_t)E &= (P + r_1)E = 0\ (mod\, \mathcal{C}^\infty) \\ Q_2(r^t - is^t - \partial_t)E &= (P + r_1^t)E = 0\ (mod\, \mathcal{C}^\infty) \end{aligned}$$

by Lemma 3.27, the proof of Theorem 3.15 applies also to this case where the wave operator factorizes only up to smoothing operators.
Thus, summing up, we have proven the following theorem:

Theorem 3.28 *Let $(\mathcal{M},g)$ be a globally hyperbolic spacetime with spacelike Cauchy surface Σ and unit-normalfield n^α.*
In a neighborhood of Σ let the pseudodifferential operators I and R be given ($mod\, S^{-\infty}$) by the equations (3.94)–(3.96), (3.91)–(3.92) and (3.87).
Then

$$\Lambda_\Sigma^{(2)}(h_1,h_2) := \frac{1}{2}\left\langle (R - iI - n^\alpha\nabla_\alpha)Eh_1, I^{-1}(R - iI - n^\alpha\nabla_\alpha)Eh_2\right\rangle_{L^2_{\mathbb{C}}(\Sigma,d^3\sigma)}$$

($h_1,h_2 \in \mathcal{D}(\mathcal{M})$) defines a Hadamard Fock state of the Klein-Gordon quantum field on $(\mathcal{M},g)$.

Remarks:

1. Our construction depends on

   - the choice of Cauchy surface Σ,
   - the choice of the vectorfield n^α: in a general spacetime the choice of the normalfield on Σ seems to be the most natural one, but on spacetimes with certain symmetries one might take other appropriate timelike vectorfields (on a stationary spacetime e.g. the Killing field),
   - the modification of $s(t,x,\xi)$ in (3.95) to make I positive,
   - the choices of operators R and I which were only defined modulo $S^{-\infty}$.

2. If we break off the asymptotic expansion of the operators s and r in equ. (3.94) at a finite value of ν, then our conjecture is that we obtain a state which is – if not an Hadamard state – at least locally quasiequivalent to one.

3. Our construction was purely local, we did not use any global properties of the spacetime $(\mathcal{M},g)$ apart from the existence of the fundamental solution E. Therefore, we can also construct local states in globally hyperbolic submanifolds of a non-globally hyperbolic

spacetime $(\mathcal{M}, g)$. We could e.g. take a double-cone region $\mathcal{N}$ with base Σ such that $\mathcal{N} = D(\Sigma)$. Then, $(\mathcal{N}, g)$ is globally hyperbolic with Cauchy surface Σ, the fundamental solution $E_{\mathcal{N}}$ of the Klein-Gordon equation in $\mathcal{N}$ exists and our construction yields states for observables localized in $\mathcal{N}$.

Our construction is reminiscent of the adiabatic DeWitt-Schwinger expansion of the Feynman propagator (see e.g. [5]) which is used for regularizing the expectation value of the energy-momentum tensor, but whereas there it is not clear that one ends up with a state (positivity is not under control), one obtains here a manifestly positive functional. It would be interesting to investigate whether our treatment could be used to set up a similar regularization procedure for the stress-energy tensor.
As we have already mentioned, not many explicit examples for Hadamard states are known. The spacetimes most frequently considered as backgrounds are the black hole spacetimes (Schwarzschild, Kerr,...). Whereas for the Schwarzschild spacetime quite a lot is known (due to the existence of a static Killing field) it seems that the only (rigorous) result for the (non-stationary) Kerr spacetime is the statement [38] that no stationary Hadamard state can exist there. It should have become clear that our work supplies methods to deal with the problem of constructing non-stationary states and it would be interesting to see how the Hawking radiation comes out in this case.
Another possible direction for future research is the extension of the whole story to spinor fields. But more interesting and promising seems to be the investigation of the new wavefront set spectrum condition proposed in [7] which is supposed to be a selection criterion for interacting field theories. One could ask how a free state gets perturbed when interaction is switched on and set up a perturbation scheme within this frame. A possible application would be to look how the thermal Hawking radiation changes in the presence of interaction.
At any rate it should have become clear that the wavefront sets and the mathematical microlocal techniques are the correct language to describe physical phenomena of quantum fields in gravitational background fields and we think that new and exciting results are to be expected from these ideas.

Acknowledgment

I thank Prof. K. Fredenhagen for a careful reading of the manuscript and useful discussions. I am particularly indebted to Marek Radzikowski who made the results of his PhD thesis available prior to publication and helped me during his visit in Hamburg a lot to understand wavefront sets. These discussions finally lead to the results of this work.
Thanks are also due to all my friends and colleagues in the "algebraic group", at the II. Institut, at DESY and outside, but in particular to Martin Köhler and Rainer Verch for numerous discussions and assistance in all mathematical or computer problems.
I feel deeply obliged to the Studienstiftung des deutschen Volkes which supported me so generously over many years. Financial support from the DFG is also gratefully acknowledged.
Finally I want to thank Cathérine for her encouragement and patience.

Appendix A

Notation and conventions

In this appendix we want to fix our notation and conventions used throughout this work.
$\mathbf{R}^n$: n-dim. real (Euclidean) space
$x = (x^1, \ldots, x^n)$, $\xi = (\xi_1, \ldots, \xi_n)$: coordinates of $\mathbf{R}^n$ resp. its dual space
$x\xi = x^1\xi_1 + \ldots + x^n\xi_n$: scalar product in $\mathbf{R}^n$
$|\xi| = [\xi_1^2 + \ldots + \xi_n^2]^{1/2}$
$\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbf{N}_o^n$: multiindex
$|\alpha| = \alpha_1 + \ldots + \alpha_n$: length of multiindex α
$\alpha! = \alpha_1! \cdot \ldots \cdot \alpha_n!$
$x^\alpha = (x^1)^{\alpha_1} \cdot \ldots \cdot (x^n)^{\alpha_n}$, $\xi^\alpha = (\xi_1)^{\alpha_1} \cdot \ldots \cdot (\xi_n)^{\alpha_n}$ for $x, \xi \in \mathbf{R}^n$
$D_x^\alpha = \left(\frac{1}{i}\frac{\partial}{\partial x^1}\right)^{\alpha_1} \cdot \ldots \cdot \left(\frac{1}{i}\frac{\partial}{\partial x^n}\right)^{\alpha_n}$ with $i = \sqrt{-1}$
$D_\xi^\alpha = \left(\frac{1}{i}\frac{\partial}{\partial \xi_1}\right)^{\alpha_1} \cdot \ldots \cdot \left(\frac{1}{i}\frac{\partial}{\partial \xi_n}\right)^{\alpha_n}$
supp f: the support of the function f, i.e. the closure of the set of points at which f does not vanish
X an open subset of $\mathbf{R}^n$
$\mathcal{E}(X) \equiv \mathcal{C}^\infty(X)$: space of smooth (infinitely differentiable) functions $f : X \to \mathbf{C}$ with locally convex topology generated by the family of seminorms $p_{n,K}(f) := \max_{x\in K} \sum_{|\alpha|\leq n} |D_x^\alpha f(x)|$ for compact subsets $K \subset X$.
$\mathcal{E}'(X)$: dual space of $\mathcal{E}(X)$ w.r.t. this topology, i.e. the continuous linear maps $\mathcal{E}(X) \to \mathbf{C}$. It is the space of distributions with compact support.
$\mathcal{D}(X) \equiv \mathcal{C}_o^\infty(X) = \{f \in \mathcal{C}^\infty(X);\ supp\, f \text{ compact}\}$: space of testfunctions with the inductive limit topology induced from $\mathcal{E}(K_i)$ for compact sets $K_i \to X$.
$\mathcal{D}'(X)$: dual space of $\mathcal{D}(X)$, the space of distributions in X
$\mathcal{S}(\mathbf{R}^n)$: Schwartz space of functions in $\mathcal{C}^\infty(\mathbf{R}^n)$ that are rapidly decaying, i.e. for any pair of integers $n, N \geq 0$ are the seminorms $p_{n,N}(f) = \sup_{x\in\mathbf{R}^n} \left[(1+|x|)^N \sum_{|\alpha|\leq n} |D_x^\alpha f(x)|\right]$ finite.
$\mathcal{S}'(\mathbf{R}^n)$: the dual space of $\mathcal{S}(\mathbf{R}^n)$ w.r.t. the locally convex topology generated by these seminorms. It is the space of tempered distributions.
Since $\mathcal{D}(\mathbf{R}^n) \subset \mathcal{S}(\mathbf{R}^n) \subset \mathcal{E}(\mathbf{R}^n)$ we have $\mathcal{E}'(\mathbf{R}^n) \subset \mathcal{S}'(\mathbf{R}^n) \subset \mathcal{D}'(\mathbf{R}^n)$.
singsupp u: the singular support of $u \in \mathcal{D}'(X)$, i.e. the smallest closed set in the complement of which u is a $\mathcal{C}^\infty$-function.
The Fourier transformation $u(x) \mapsto \hat{u}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} e^{-ix\xi} u(x)\, d^n x$ is an isomorphism of $\mathcal{S}(\mathbf{R}^n)$

onto $\mathcal{S}(\mathbf{R}^n)$, its inverse is given by $\hat{u}(\xi) \mapsto u(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbf{R}^n} e^{ix\xi} \hat{u}(\xi)\, d^n\xi$.
$\mathcal{E}(\mathcal{M})$, $\mathcal{D}(\mathcal{M})$, $\mathcal{E}'(\mathcal{M})$, $\mathcal{D}'(\mathcal{M})$ can be analogously defined on a manifold $\mathcal{M}$ by localization, whereas $\mathcal{S}$ and $\mathcal{S}'$ in general not.
$\mathcal{M}$ is a (4-dim.) paracompact $\mathcal{C}^\infty$-manifold endowed with a Lorentzian metric g of signature $(+---)$. Units are chosen such that $\hbar = c = G = k_B = 1$.
$(\mathcal{M}, g)$ is time-orientable if there exists a smooth timelike vector field on $\mathcal{M}$, i.e. we can unambiguously distinguish the future light cone from the past light cone throughout the manifold.
$(\mathcal{M}, g)$ is globally hyperbolic if it possesses a Cauchy surface Σ, i.e. a 3-dim. hypersurface that is intersected by each inextendible causal (null or timelike) curve in $\mathcal{M}$ exactly once. Equivalently, $(\mathcal{M}, g)$ possesses a foliation $\mathcal{M} = \mathbf{R} \times \Sigma$ into hypersurfaces Σ such that $\Sigma_t = \{t\} \times \Sigma$ is a spacelike Cauchy surface for $(\mathcal{M}, g)$. In this work we always understand a globally hyperbolic manifold as being time-orientable.
If S is a subset of $\mathcal{M}$, we define $J^+(S)$ (resp. $J^-(S)$) to be the set of all points $x \in \mathcal{M}$ such that x can be connected to a point in S by a future-directed (resp. past-directed) causal curve from S to x in $\mathcal{M}$, and $D^+(S)$ (resp. $(D^-(S))$ the set of all points $x \in J^+(S)$ (resp. $J^-(S)$) such that every past- (resp. future-) directed inextendible causal curve through x passes through S. $D(S) := D^+(S) \cup D^-(S)$ is called the domain of dependence of S.
A convex normal neighborhood in $\mathcal{M}$ is an open set $U \subset \mathcal{M}$ s.th. for any two points $x_1, x_2 \in \mathcal{M}$ there exists a unique geodesic contained in U which connects x_1 and x_2.
$\sigma(x_1, x_2) = \pm \left(\int_a^b \left| g_{\mu\nu}(x(\tau)) \frac{dx^\mu}{d\tau} \frac{dx^\nu}{d\tau} \right|^{1/2} d\tau \right)^2$ is the square of the geodesic distance from x_1 to x_2 in a convex normal neighborhood U, where $[a, b] \to \mathcal{M}, \tau \mapsto x(\tau)$ is the unique geodesic curve in U from x_1 to x_2 ($+$ ($-$) is chosen if $x(\tau)$ is spacelike (timelike)).

Bibliography

[1] S.L. Adler and J. Lieberman. Trace anomaly of the stress-energy tensor for massless vector particles propagating in a general background metric. *Ann. Phys. (NY)*, 113:294–303, 1978.

[2] S.L. Adler, J. Lieberman, and Y.J. Ng. Regularization of the stress-energy tensor for vector and scalar particles propagating in a general background metric. *Ann. Phys. (NY)*, 106:279–321, 1977.

[3] A. Ashtekar and A. Magnon. Quantum fields in curved space-times. *Proc. Roy. Soc. A*, 346:375–394, 1975.

[4] D. Bernard. Hadamard singularity and quantum states in Bianchi type-I space-time. *Phys. Rev. D*, 33:3581–3589, 1986.

[5] N.D. Birrell and P.C.W. Davis. *Quantum Fields in Curved Space*. Cambridge Univ. Press, Cambridge, 1982.

[6] D.G. Boulware. Quantum field theory in Schwarzschild and Rindler spaces. *Phys. Rev. D*, 11:1404–1423, 1975.

[7] R. Brunetti, K. Fredenhagen, and M. Köhler. The wave front set spectrum condition and Wick ordered products of free fields on a manifold. In Preparation, 1995.

[8] P.R. Chernoff. Essential self-adjointness of powers of generators of hyperbolic equations. *J. Funct. Anal.*, 12:401–414, 1973.

[9] P. Chmielowski. States of scalar fields on spacetimes with two isometries with timelike orbits. *Class. Quantum Grav.*, 11:41–56, 1994.

[10] S.M. Christensen. Vacuum expectation value of the stress tensor in an arbitrary curved background: The covariant point-separation method. *Phys. Rev. D*, 14:2490–2501, 1976.

[11] D. Deutsch and A.-H. Najmi. Construction of states for quantum fields in nonstatic space-times. *Phys. Rev. D*, 28:1907–1915, 1983.

[12] B.S. DeWitt and R.W. Brehme. Radiation damping in a gravitational field. *Ann. Phys. (NY)*, 9:220–259, 1960.

[13] J. Dimock. Algebras of local observables on a manifold. *Comm. Math. Phys.*, 77:219–228, 1980.

[14] J. Dimock and B.S. Kay. Classical and quantum scattering theory for linear scalar fields on the Schwarzschild metric II. *J. Math. Phys.*, 27:2520–2525, 1986.

[15] J. Dimock and B.S. Kay. Classical and quantum scattering theory for linear scalar fields on the Schwarzschild metric I. *Ann. Phys. (NY)*, 175:366–426, 1987.

[16] J.J. Duistermaat and L. Hörmander. Fourier integral operators II. *Acta Math.*, 128:183–269, 1972.

[17] K. Fredenhagen and R. Haag. Generally covariant quantum field theory and scaling limits. *Comm. Math. Phys.*, 108:91–115, 1987.

[18] K. Fredenhagen and R. Haag. On the derivation of Hawking radiation associated with the formation of a black hole. *Comm. Math. Phys.*, 127:273–284, 1990.

[19] S.A. Fulling. Nonuniqueness of canonical field quantization in Riemannian space-time. *Phys. Rev. D*, 7:2850–2862, 1973.

[20] S.A. Fulling. Remarks on positive frequency and Hamiltonians in expanding universes. *Gen. Rel. Grav.*, 10:807–824, 1979.

[21] S.A. Fulling. *Aspects of Quantum Field Theory in Curved Space-Time.* Cambridge University Press, Cambridge, 1989.

[22] S.A. Fulling, F.J. Narcowich, and R.M. Wald. Singularity structure of the two-point function in quantum field theory in curved spacetime, II. *Ann. Phys. (NY)*, 136:243–272, 1981.

[23] S.A. Fulling, M. Sweeny, and R.M. Wald. Singularity structure of the two-point function in quantum field theory in curved spacetime. *Comm. Math. Phys.*, 63:257–264, 1978.

[24] R. Haag. *Local quantum physics: Fields, particles, algebras.* Springer Verlag, Berlin, 1992.

[25] R. Haag, N.M. Hugenholtz, and M. Winnink. On the equilibrium states in quantum statistical mechanics. *Comm. Math. Phys.*, 5:215–236, 1967.

[26] R. Haag and D. Kastler. An algebraic approach to quantum field theory. *J. Math. Phys.*, 5:848–861, 1964.

[27] R. Haag, H. Narnhofer, and U. Stein. On quantum field theory in gravitational background. *Comm. Math. Phys.*, 94:219–238, 1984.

[28] J.B. Hartle and S.W. Hawking. Path integral derivation of black hole radiance. *Phys. Rev. D*, 13:2188–2203, 1976.

[29] S.W. Hawking. Particle creation by black holes. *Comm. Math. Phys.*, 43:199–220, 1975.

[30] H.J. Heßling. *Quanten-Äquivalenzprinzip.* PhD thesis, Universität Hamburg, September 1992.

[31] L. Hörmander. Fourier integral operators I. *Acta Math.*, 127:79–183, 1971.

[32] B.S. Kay. Linear spin-zero quantum fields in external gravitational and scalar fields. *Comm. Math. Phys.*, 62:55–70, 1978.

[33] B.S. Kay. A uniqueness result in the Segal-Weinless approach to linear Bose fields. *J. Math. Phys.*, 20:1712–1713, 1979.

[34] B.S. Kay. The double-wedge algebra for quantum fields on Schwarzschild and Minkowski spacetimes. *Comm. Math. Phys.*, 100:57–81, 1985.

[35] B.S. Kay. A uniqueness result for quasi-free KMS states. *Helv. Phys. Acta*, 58:1017–1029, 1985.

[36] B.S. Kay. Quantum field theory in curved spacetime. In K. Bleuler and M. Werner, editors, *Differential geometrical methods in theoretical physics*, pages 373–393. Kluwer Acad. Publ., 1988.

[37] B.S. Kay. Sufficient conditions for quasifree states and an improved uniqueness theorem for quantum fields on space-times with horizons. *J. Math. Phys.*, 34:4519–4539, 1993.

[38] B.S. Kay and R.M. Wald. Theorems on the uniqueness and thermal properties of stationary, nonsingular, quasifree states on spacetimes with a bifurcate Killing horizon. *Phys. Rep.*, 207:49–136, 1991.

[39] M. Köhler. New examples for Wightman fields on a manifold. *DESY–Preprint 94–161; Submitted to Class. and Quant. Grav.*, 1994.

[40] M. Köhler. *The stress energy tensor of a locally supersymmetric quantum field on a curved spacetime.* PhD thesis, Universität Hamburg, April 1995.

[41] C. Lüders and J.E. Roberts. Local quasiequivalence and adiabatic vacuum states. *Comm. Math. Phys.*, 134:29–63, 1990.

[42] J. Manuceau and A. Verbeure. Quasi-free states of the C.C.R.-algebra and Bogoliubov transformations. *Comm. Math. Phys.*, 9:293–302, 1968.

[43] F.D. Mazzitelli, J.P. Paz, and M.A. Castagnino. Cauchy data and Hadamard singularities in time-dependent backgrounds. *Phys. Rev. D*, 36:2994–3001, 1987.

[44] A.-H. Najmi and A.C. Ottewill. Quantum states and the Hadamard form. III. Constraints in cosmological space-times. *Phys. Rev. D*, 32:1942–1948, 1985.

[45] L. Parker. Quantized fields and particle creation in expanding universes. I. *Phys. Rev.*, 183:1057–1068, 1969.

[46] L. Parker. Quantized fields and particle creation in expanding universes. II. *Phys. Rev. D*, 3:346–356, 1971.

[47] L. Parker and S.A. Fulling. Adiabatic regularization of the energy-momentum tensor of a quantized field in homogeneous spaces. *Phys. Rev. D*, 9:341–354, 1974.

[48] K.-T. Pirk. Hadamard states and adiabatic vacua. *Phys. Rev. D*, 48:3779–3783, 1993.

[49] M.J. Radzikowski. *The Hadamard condition and Kay's conjecture in (axiomatic) quantum field theory on curved space-time.* PhD thesis, Princeton University, October 1992.

[50] M. Reed and B. Simon. *Methods of Modern Mathematical Physics II.* Academic Press Inc. London, 1975.

[51] R.T. Seeley. Complex powers of an elliptic operator. *Am. Math. Soc. Proc. Symp. Pure Math.*, 10:288–307, 1968.

[52] M.E. Taylor. *Pseudodifferential Operators.* Princeton University Press, Princeton, New Jersey, 1981.

[53] W.G. Unruh. Notes on black hole evaporation. *Phys. Rev. D.*, 14:870–892, 1976.

[54] R. Verch. Antilocality and a Reeh-Schlieder theorem on manifolds. *Lett. Math. Phys.*, 28:143–154, 1993.

[55] R. Verch. Local definiteness, primarity and quasiequivalence of quasifree Hadamard quantum states in curved spacetime. *Comm. Math. Phys*, 160:507–536, 1994.

[56] R.M. Wald. The back reaction effect in particle creation in curved spacetime. *Comm. Math. Phys.*, 54:1–19, 1977.

[57] R.M. Wald. Trace anomaly of a conformally invariant quantum field in curved spacetime. *Phys. Rev. D*, 17:1477–1484, 1978.

[58] R.M. Wald. On the Euclidean approach to quantum field theory in curved spacetime. *Comm. Math. Phys.*, 70:221–242, 1979.

[59] R.M. Wald. *General Relativity.* The University of Chicago Press, Chicago, 1984.